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USERS' MANUAL FOR SHARC-3, STRATEGIC HIGH-ALTITUDE RADIANCE CODE

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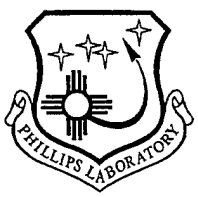
21 May 1996



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13. ABSTRACT *(Maximum 200 words)*

The Strategic High-Altitude Radiance Code, SHARC-3, calculates atmospheric radiance and transmission over a 1 - 40 μm spectral region for arbitrary lines of sight (LOS) between 50 and 300 km altitude. It models radiation due to non local thermodynamic equilibrium (NLTE) molecular emissions, the dominant sources at these altitudes. This third release of SHARC has been upgraded to model LOS's across and near the atmospheric terminator. It interpolates between several atmospheric profiles, which represent variations in species concentration through that region. In addition the spectral distribution of sunlight which has passed through the lower atmosphere is approximated by a series of optical depth functions for that part of the solar path below 50 km altitude. Auxiliary atmospheric profile generator and slit function programs enhance the capabilities of the code. Data for the previously supported major radiators have been upgraded where necessary, and CH_4 and minor isotopes of H_2O have been added. As before, auroral regions can be embedded in quiescent atmospheres, and industry-standard kinetics and radiation transport modules have been employed. This manual outlines the scientific basis of the code, details steps for code installation and use as supplied, and indicates how the user may modify the supplied chemistry if desired.

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1. INTRODUCTION

This manual describes SHARC-3, the third major release of the Strategic High-Altitude Radiance Code. It briefly discusses the underlying phenomenology and aids the user in running SHARC-3 by providing code implementation instructions and illustrative interactive sessions. As with its two previous releases,[1,2] SHARC-3 predicts infrared (IR) atmospheric radiation and transmittance in the 1-40 μm spectral region and includes important bands of NO, CO, H_2O, O_3, OH, CO_2, CH_4, and NO^+. Several upgrades and new features have been added to this version; they include:

- the atmosphere can now be partitioned into as many as five distinct regions which are called extended (one) and local regions (the rest);
- each region can have up to seven different atmospheric profiles tied to specific solar zenith angles;
- the model now incorporates arbitrary paths around and across the solar terminator;
- methane (CH_4) and minor isotopes of H_2O have been added to the species which SHARC currently supports;
- the database of atmospheric lines has been recalculated using the HITRAN 92 line atlas supplemented with additional lines for O_3, NO and NO^+; and
- an external, empirical, database-driven SHARC Atmospheric Generator (SAG) has been added to provide atmospheric profiles as a function of time, date, location and geomagnetic activity.

These upgrades allow SHARC to simulate the effects of changing atmospheric composition and temperature around the solar terminator. This manual discusses these new features and reviews other capabilities which SHARC-3 has in common with its predecessors.

SHARC-3 was developed as a modular code so that models and model parameters can be easily modified or upgraded as additional data and/or better models become available.[3] The present modules include input, ambient chemistry, time-dependent auroral chemistry, radiative transport, geometry, and output. The input module is interactive, menu-driven, and checks all input parameters for validity before continuing with the calculation. An ongoing upgrade, to appear in a future release, is the development of a two-temperature rotational distribution for OH and NO, motivated by results from the CIRRIS 1A experiment.[4,5]

The calculational sequence for a line-of-sight (LOS) radiance calculation which passes through an auroral region involves the following steps. First the input module prepares the inputs required by the

rest of the code. The next step is calculation of the excited-state populations. This is accomplished in the chemistry modules: ambient and auroral. The ambient population module iterates between a generalized chemical kinetics module[6] that calculates excited-state populations due to solar and earthshine excitation and a Monte-Carlo based radiative transfer model[7] that calculates radiative excitation and energy transfer between atmospheric layers. The molecular line parameters are taken from the 1992 HITRAN line atlas[8] and supplemented with additional lines for the high vibrational states of NO, $O_3(\nu_3)$ and NO^+.

Starting with a set of ambient populations, the auroral module calculates the NLTE population enhancements caused by the flux of high energy electrons. The geometry module determines the species column densities for each layer traversed by the user's requested path. The radiative transport module then calculates the radiance along the path for each molecular excited state. The calculation is done on a line-by-line (LBL) basis in that the total radiation from each line is calculated using a single-line equivalent-width formulation that incorporates a Doppler-Lorentz (Voigt) line shape.

A general discussion of atmospheric radiation at high altitudes and the important infrared-active molecules is given in the next section, with an overview of SHARC in Section 3. Sections 4-7 provide information on how to run SHARC, its output files, its input files, and the auxiliary programs associated with it. Various user instructions, supplemental information and a sample output are given in the appendices.

2. HIGH-ALTITUDE INFRARED RADIATION CONCEPTS

2.1 Non Local Thermodynamic Equilibrium Conditions

Before discussing IR radiators in the upper atmosphere, we introduce the very important concept of non local thermodynamic equilibrium (NLTE). Figure 1 shows the number of collisions a molecule suffers per second as a function of altitude. The relevant inputs, density, temperature, etc., are taken from the U.S. Standard Atmosphere. The number of collisions decreases rapidly as a function of altitude.[9] This fact influences the high-altitude IR airglow in a profound way. This can be seen as follows: At steady state the ratio of the density of a vibrationally excited species [M^*] to the density of its ground state [M] is given by

$$[M^*]/[M] = \frac{P_c + J}{L_c + A} \quad , \tag{1}$$

where P_c and L_c are the terms for production and loss, respectively, of M^* due to collisions. J is the radiative pumping term due to absorption of radiation from earthshine, sunshine and the atmosphere, and A is the radiative loss term or the Einstein A Coefficient for spontaneous emission. At lower altitudes, the collisional production and loss processes are much faster than the radiative ones,

$$[M^*]/[M] = P_c/L_c = Equilibrium\ Constant(K) \tag{2}$$

and local thermodynamic equilibrium (LTE) holds. Under these conditions IR airglow emitted by M^* can be described by the black body laws at the local thermal equilibrium temperature. When the radiative terms are not negligible compared to the collisional terms and Equation (2) can no longer be used to describe the situation, thermodynamic equilibrium no longer prevails. The situation is described as NLTE. A rule of thumb is that the radiation begins to deviate from LTE when there are less than a million collisions per radiative lifetime. The radiative lifetime of the v=1 state of NO is about 0.1 s, so the 5.3 μm radiation from NO begins to deviate from equilibrium around 40 km altitude. This is an approximate but helpful rule which is applicable to species that are not produced by chemiluminescence or photodissociation. An exception to this rule of thumb is the 15 μm band of CO_2. Due to fast pumping during collisions with oxygen atoms,[10,11] this mode stays in equilibrium up to above 100 km altitude.[12] At very high altitudes the radiative pumping and loss terms J and A in Equation (1) are much larger than the collisional pumping and loss terms P_c and L_c. The ratio of the excited to ground state densities then becomes

$$[M^*] / [M] = J/A \quad . \tag{3}$$

This situation is described as "radiative equilibrium". At altitudes greater than about 150 km the ratio of the densities of the CO_2 vibrational levels 01^101 and 00^001 is determined solely by the upwelling earthshine. The frequency of collisions is too small to have any impact.

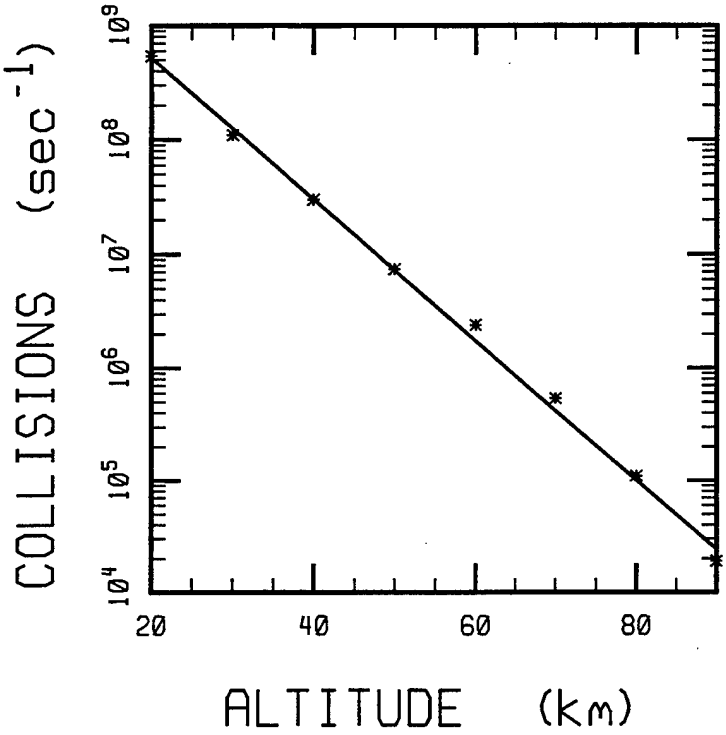

Figure 1. The Number of Collisions Suffered by an Atom or Molecule Per Second as a Function of Altitude.[9]

The arguments cited above apply to stable species for which normally only the lowest vibrational level is populated and which may be excited by earthshine, sunshine, and collisions. They are not applicable to the species produced by chemiluminescence (OH and O_3) and by photodissociation (the singlet delta excited electronic state, $^1\Delta_g$, of O_2). In such cases the pumping and loss terms in Equation (1) become more complicated because vibrationally excited levels may be populated by chemical reactions or by photodissociation, and these levels can influence the production or loss processes of other levels. We then have a number of coupled equations instead of the simple Equation (1). Nevertheless, Equation (1) nicely illustrates the basic points involved in calculating the ratio of the excited (upper) to ground (lower) state density.

2.2 Vibrational Temperature

At this point it is useful to introduce the concept of a vibrational temperature. This concept is based upon the experimental observation that translation to vibration (T-V) energy transfer rate coefficients are usually much smaller than translation to rotation (T-R) rates or the near resonant vibration to vibration (V-V) rates. Whereas T-V and T-R rates equilibrate translational degrees of freedom with vibrational and rotational degrees of freedom respectively, the V-V near resonant rates lead to the establishment of a Maxwell-Boltzmann distribution in a given vibrational manifold. We then have a situation where the translational and rotational degrees of freedom can be described by one temperature and the vibrational levels are described by an entirely different temperature. Of course two different vibrational manifolds in the same molecule may be described by two different vibrational temperatures. For example, the ν_2 and ν_3 vibrational fundamental states of CO_2 in NLTE situations invariably have different vibrational temperatures. If two vibrational modes are coupled by the Fermi or Dennison resonances, they may rapidly equilibrate and have the same vibrational temperatures. Again, the ν_1 and ν_2 modes of CO_2 coupled by their Fermi resonance are believed to have the same vibrational temperature. The vibrational temperature T_v is defined by the relation

$$T_v = c_2 E / [\ln(g_e n_\ell / g_\ell n_e)] \quad , \tag{4}$$

where g_e and g_ℓ are the statistical weights of the excited and lower states, and n_e and n_ℓ are their respective number densities. E is the vibrational spacing between the two levels in cm^{-1}, and $c_2 = 1.4388$ K/cm^{-1} is the second radiation constant. The temperature or population of the upper state is usually defined relative to the population of the ground state, that is, ℓ is the ground state. It is clear from Equation (4) that T_v becomes equal to the translational temperature T when thermodynamic equilibrium prevails. Defining a vibrational temperature has proven to be a useful concept because it not only indicates departure from equilibrium but also the extent of this departure.

Up to now the SHARC model has assumed that rotational degrees of freedom are in equilibrium with translational motion. However, CIRRIS 1A results have shown that the rotational states of nighttime OH[4] and daytime and aurorally produced NO[5] are not in equilibrium. Ongoing work is focussing on modeling these phenomena with a two-temperature rotational distribution, to be included in future releases of SHARC.

The lack of collisions leads to a departure from equilibrium (NLTE situations), but more frequent collisions do not guarantee thermodynamic equilibrium. This point is illustrated by the solar pumped

airglow which, for bands like the 2.7 μm CO_2, can establish a steady state population of excited molecular levels higher than those given by LTE as far down as 50 km altitude.

2.3 Molecular Radiators

Currently SHARC supports the major isotope for NO, O_3, H_2O, CO, OH, CH_4, CO_2, and NO^+. Also the important minor isotopes of CO_2 and H_2O are included. We define natural conditions to be the quiescent and aurorally disturbed atmosphere. Atmospheric radiation in this wavelength interval arises from either vibration-rotation (V-R) transitions of these molecules or from pure rotational transitions of OH and H_2O. Pure rotational transitions of NO, CO, and O_3 occur farther towards the red, around 100 μm, because these molecules have large moments of inertia; the pure rotational transitions for CO_2 are unallowed because it has no permanent dipole moment. The most abundant species, N_2 and O_2, have no IR vibration-rotation or pure rotational spectra because they have neither transitions nor permanent dipole moments.

The primary source of information about the intensity and location of the spectral lines is the HITRAN data tape.[8] It contains virtually all of the important lines for LTE conditions. Additional lines were added for NLTE transitions from the higher vibrational levels of $O_3(\nu_3)$.[13] Supplementary data were also obtained for NO,[14] and for NO^+.[15] For OH, HITRAN line locations were used, but line strengths were derived from a recent study.[16] The total intensity of the various bands are given by their usual Einstein A coefficients, which are derived by a properly weighted average of the A coefficients of the individual V-R transitions.[15]

2.3.1 CO_2

Figure 2 shows the important CO_2 transitions observed in the infrared. There are three sets of strong transitions, which result in bands around 15.0, 4.3, and 2.7 μm. The relative strengths of the most important bands of these transitions are determined from their Einstein A coefficients. Some illustrative SHARC-3 values for the most common isotope are given in Table 1.

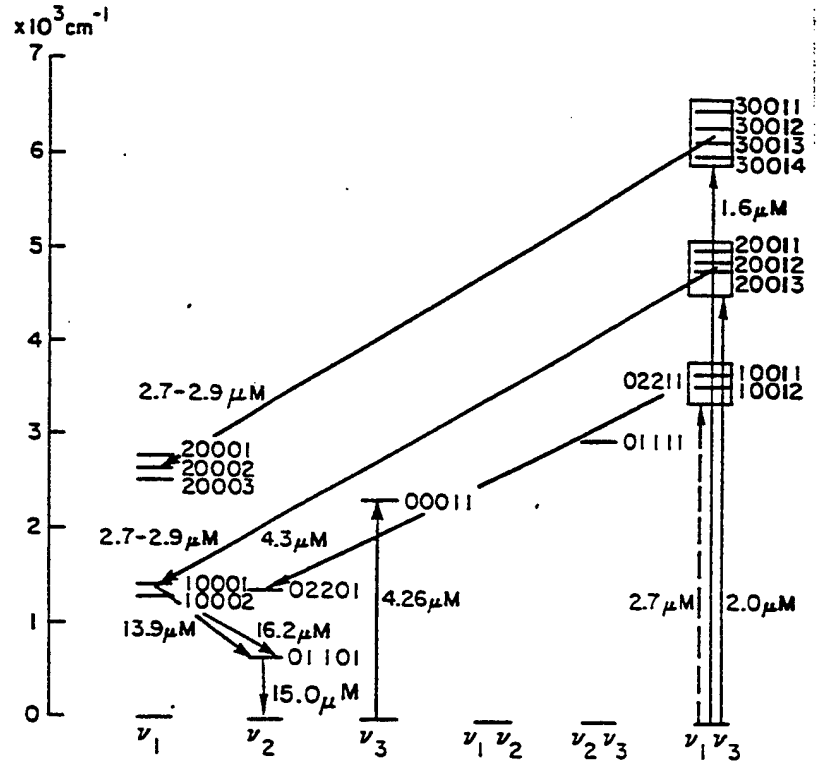

Figure 2. Important CO_2 Airglow Transitions and their Energy Levels.

Table 1. Illustrative Einstein A Coefficients for CO_2.

Upper State	Lower State	Energy (cm^{-1})	Einstein A Coefficient (s^{-1})
$10^{0}02$	$01^{1}01$	618.	1.148
$01^{1}01$	$00^{0}01$	667.4	1.500
$02^{2}01$	$01^{1}01$	667.8	1.17
$10^{0}01$	$01^{1}01$	721.	1.566
$00^{0}11$	$10^{0}01$	961.	0.442
$00^{0}11$	$10^{0}02$	1064.	0.467
$00^{0}11$	$00^{0}01$	2349.	432.95
$10^{0}12$	$00^{0}01$	3613.	11.15
$10^{0}11$	$00^{0}01$	3715.	17.92

Around 15 μm, the bands result from a change of one quantum of bending mode ν_2. These transitions are very prominent in the emission from the earth's atmosphere, and the sharp Q-branch can be clearly seen in spectra of the earth taken at spectral resolutions of a few wavenumbers from a balloon, rocket or satellite.[17,18] The reason for this is very simple. The spectrum of a 300 K blackbody peaks near 10 μm. Therefore, there are large numbers of 15 μm photons in the radiation, termed earthshine, emitted by the earth's atmosphere as well as by the earth itself. Since the 15 μm CO_2 band is very strong, its

transitions to the ground state and low lying excited states are severely self-absorbed. This fact has important consequences for atmospheric radiation which we will point out as we go along. Similarly, solar radiation has negligible influence on the 15 μm radiation because of the small number of solar photons at this wavelength. The intensity of 15 μm radiation therefore shows no diurnal variation.[14] The second band, around 4.3 μm, arises from the emission of a quantum from the asymmetric stretch ν_3. Because earthshine does not contain a strong 4.3 μm component, this band is much stronger during daytime. Solar radiation at 4.3 μm, 2.7 μm, 2.0 μm, and 1.6 μm is absorbed followed by a large probability of emission at 4.3 μm.[19] The probability of emission is largest at 4.3 μm because of the much larger Einstein A coefficients (Table 1) than those at 2.7 μm. The probability of re-emission at 2.0 and 1.6 μm is negligible because of their very small A coefficients. Transitions near 4.3 μm to the ground state and also to the low lying excited states are severely self-absorbed too. The third band, around 2.7 μm, is due to emission from the combination bands of $\nu_1+\nu_3$. This emission, even more than the 4.3 μm component, is predominantly observed from the sunlit atmosphere.

In the aurorally dosed atmosphere a large amount of emission from the ν_3 band of CO_2 around 4.3 μm is observed.[15] This emission arises from the near-resonant transfer of vibrational energy from N_2 to the ν_3 mode of CO_2. The nitrogen, in turn, is vibrationally populated by collisions with low energy secondary electrons. It takes a finite amount of time to transfer energy from N_2 to CO_2, and this time varies with altitude because of the density (see Figure 1). This CO_2 emission is called delayed emission as opposed to direct or prompt emission from an excited state of NO which is chemically created in an excited state and subsequently decays via photon emission.

2.3.2 NO

Nitric oxide is a prominent radiator in the high altitude atmosphere. The 5.3 μm emission from its (1-0) vibrational transition is the most efficient atmospheric cooling agent between about 100 and 150 km altitude. This is because collisions between NO and atomic oxygen efficiently transfer translational energy into vibrational energy. The reverse V-T process has an almost gas kinetic cross-section at room temperature. The 5.3 μm emission from NO in the thermosphere is so bright that stratospheric limb radiance calculations that do not include NO emission in the thermosphere nor the excitation of these NO bands by thermospheric emission are likely to be incorrect.

In an aurorally dosed atmosphere, NO is also produced by the reaction between N atoms and O_2. The NO thus produced may be excited to vibrational levels as high as $v=12$. The result of emission from high vibrational levels is that the fundamental band ($\Delta v=1$) is spread towards longer (red) wavelengths.

In contrast to the non-auroral atmosphere, overtone bands ($\Delta v=2$) of NO around 2.7 μm are seen. A schematic illustrating the atomic and molecular radiators produced in an auroral atmosphere is shown in Figure 3; further details are available in Reference (18).

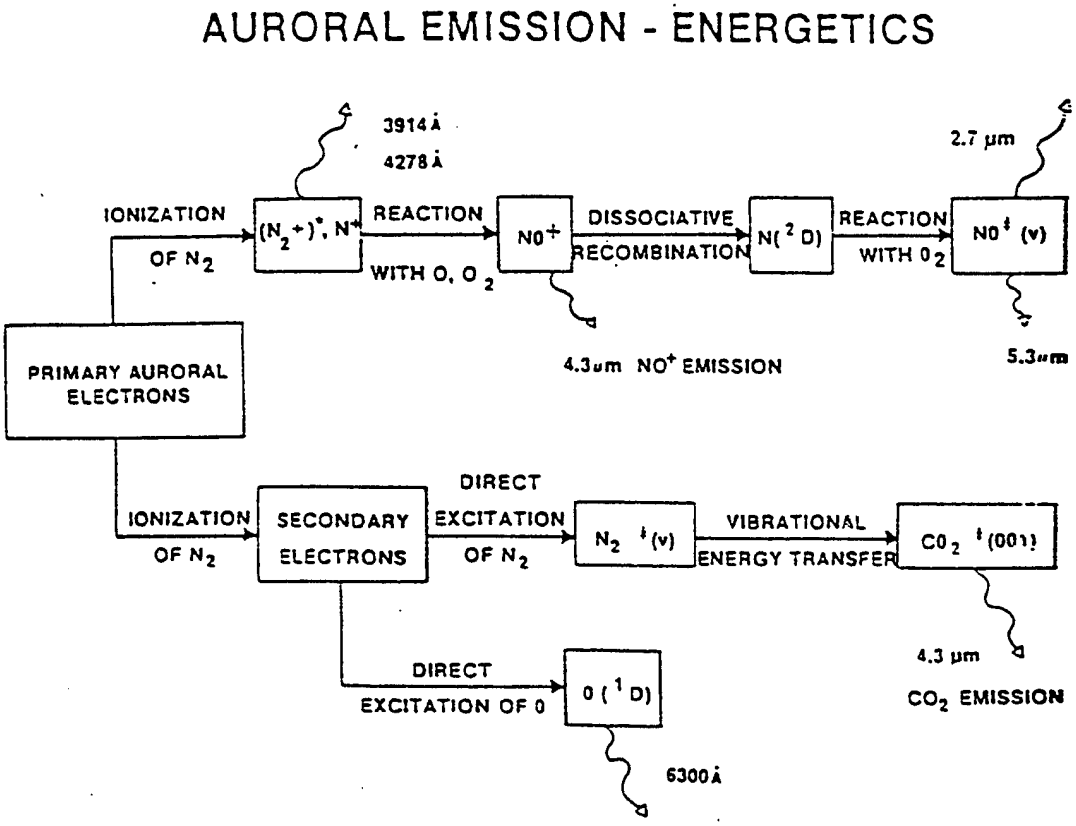

Figure 3. Illustrative Reaction Scheme Leading to Aurorally Enhanced Atmospheric IR Radiation at High Altitudes.[18]

2.3.3 O_3

The nonlinear triatomic molecule O_3 has three vibrational degrees of freedom. The vibrational mode ν_1 at 1103 cm^{-1} has an Einstein A coefficient of about 0.5 s^{-1} compared to about 10 s^{-1} for the ν_3 mode at 1042 cm^{-1} and about 0.08 s^{-1} for the ν_2 mode at 701 cm^{-1}. Because of its much larger Einstein coefficient, emission from the ν_3 mode is the dominant ozone emission observed from the earth's atmosphere. It is well known that ozone is photodissociated by the ultraviolet component of solar radiation. The three body recombination reaction $O+O_2+M \rightarrow O_3+M$ regenerates ozone during

nighttime. The ozone thus formed is in highly excited vibrational states. In the stratosphere, this newly formed ozone quickly loses its vibrational energy via collisions. However, because of the lower densities in the mesosphere, radiative processes, especially those involving the ν_3 mode, become rapid enough so that emissions from excited vibrational levels are observed in the 10-13 μm region. Identification of levels responsible for this radiation is still not complete, and considerable work needs to be done before a complete model of ozone emission in the mesosphere can be constructed. Because of the decreasing total density, the three-body recombination process becomes slower in the thermosphere, and emission from ozone decreases rapidly.

2.3.4 H_2O

Figure 4 shows the three fundamental vibration-rotation transitions of water vapor and the important combination and difference bands. Only transitions near 6.3 μm are observed in the nighttime atmosphere. Transitions near 2.7 μm and 4.85 μm originate from the vibration-rotation levels pumped by solar radiation. Vibration-rotation bands of water have a very complex rotational structure arising from the fact that water is an asymmetric top molecule with three different moments of inertia. Further, these moments of inertia are small and the fact that water has a large permanent dipole moment leads to its rich rotational spectrum in the 18-40 μm region. One possible source of excitation of these vibration-rotation levels is the accidental resonance of these levels with the nighttime emission from OH. Thus far, this source has not been shown to be the cause of any IR radiance.

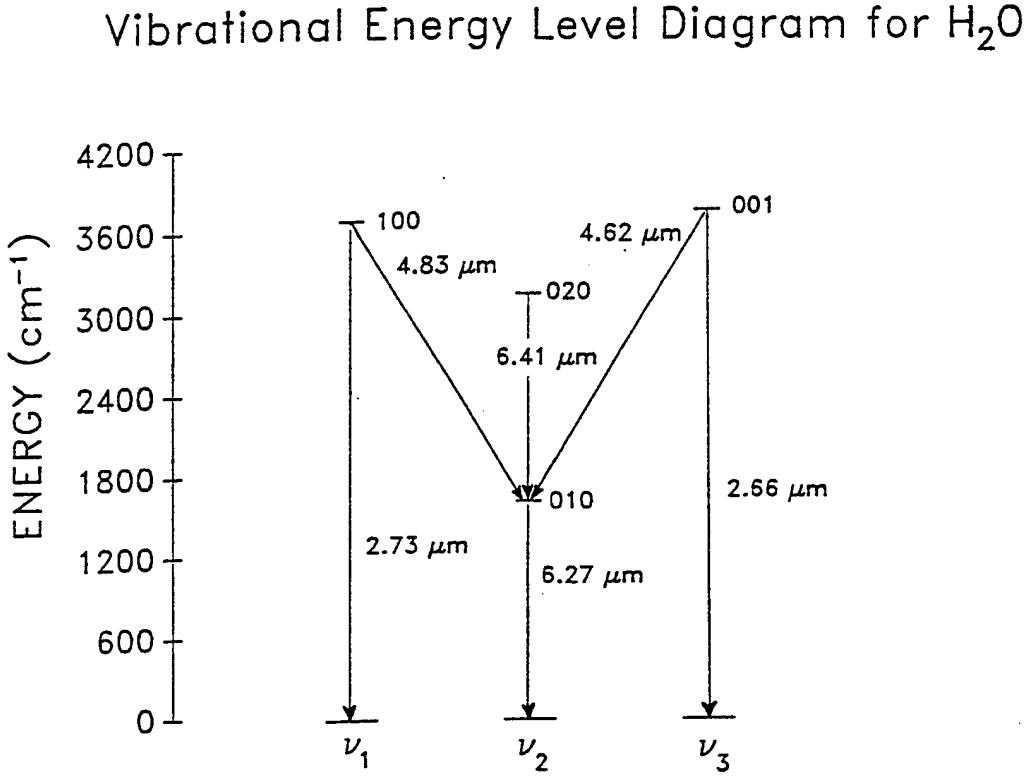

Figure 4. H_2O Transitions for the Lower Energy Levels that Contribute to Atmospheric IR Radiance at High Altitudes.

2.3.5 CO

CO is another important atmospheric radiator because of its presence up to altitudes of 300 km. It is vibrationally excited by emission from the earth's surface and emission from the stratosphere during the night; during the day excitation by sunshine leads to further enhancement. CO vibrational excitation is not as closely tied to that of N_2 as is that of asymmetric stretch ν_3 of CO_2, because of its smaller rate for transfer of vibrational energy from N_2 to CO. For this molecule, NLTE vibrational distributions exist at all altitudes.

2.3.6 OH

It is well established that the OH $\Delta v=1$ and $\Delta v=2$ emissions around 2.8 and 1.4 μm are important contributors to the near IR nighttime airglow in the 80-90 km altitude range. The OH radical is produced around 85 km primarily by the reaction[20]

$$H + O_3 \rightarrow OH + O_2 \quad , \tag{5}$$

and possibly secondarily by the reaction

$$O + HO_2 \rightarrow OH + O_2 \quad . \tag{6}$$

Both these processes produce vibrationally excited OH, with the first reaction producing excitations up to the ninth vibrational level. OH is one of very few molecules for which multiquantum radiative transitions are allowed. Thus the higher Δv transitions extend OH emissions all the way up to the visible spectral region. These vibrational transitions, for historical reasons, are called Meinel bands.[18]

2.3.7 CH_4

A preliminary chemical kinetics model for CH_4 was developed for SHARC.[21] It contains the various vibrational excitation/deexcitation mechanisms and radiative relaxation processes. The CH_4 molecule as presently included in HITRAN possesses three major groups of bands around 2.3, 3.4, and 7 μm. The states associated with these transitions are shown in Figure 5. The vibrational state designation is adapted from HITRAN, where the first, second, forth, and sixth integers represent the ν_1, ν_2, ν_3, and ν_4 vibrations, respectively. The two low lying vibrational bends (ν_2 and ν_4) comprise transitions from Group 1 states to the ground state at 6.5 and 7.6 μm, respectively. Transitions from Group 2 to the ground state involve the symmetric and asymmetric stretches at 3.4 and 3.3 μm, as well as the first overtones of ν_2 and ν_4 and the $\nu_2+\nu_4$ combination band. Of all these bands involving Group 2 states, the asymmetric stretch at 3.3 μm (ν_3) is the strongest transition. Finally, the emissions near 2.3 μm are due to transitions from Group 3 states to the ground state (the $\nu_1+\nu_4$, $\nu_3+\nu_4$, and $\nu_2+\nu_3$ combination bands), the strongest of which is the $\nu_1+\nu_4$ band.

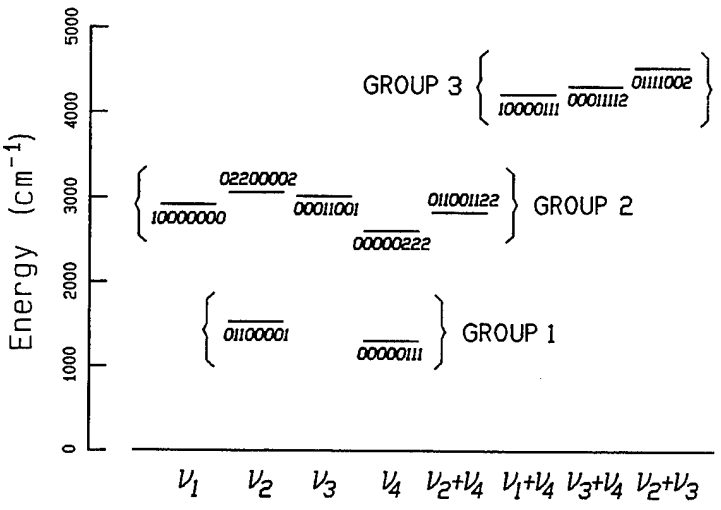

Figure 5. Vibrational Energy Level Diagram for CH_4.

The most important energy transfer processes establishing the vibrational state populations are intermolecular vibrational-to-vibrational energy exchange between CH_4 vibrational states belonging to Groups 1, 2, and 3 with ambient O_2. A summary of the CH_4 bands included in SHARC are given in Table 2. Also shown are the strengths of the vibrational transitions as indicated by the Einstein A coefficients.

CH_4 emission only makes a significant contribution to the short wavelength infrared (SWIR) emission during the daytime and to the long wavelength infrared (LWIR) during the daytime or nighttime in the lower mesosphere (around 50 km). The contributions of various molecular emissions predicted by SHARC is shown in Figure 6 for the SWIR during daytime and in Figure 7 for the LWIR during nighttime. Figure 8 shows illustrative day and night calculations for CH_4.

Table 2. Thermally Averaged Einstein A Coefficients.

TRANSITION	FREQUENCY (CM^{-1})	EINSTEIN A (S^{-1})
00000111 → 00000000	1310.761	2.23
01100001 → 00000000	1533.337	0.054
00000202 → 00000000	2596.000	0.0005
00000222 → 00000000	2612.000	0.054
01100112 → 00000000	2830.000	0.365
10000000 → 00000000	2917.000	0.005
00011001 → 00000000	3018.921	24.43
02200002 → 00000000	3062.000	0.086
10000111 → 00000000	4223.497	1.02
00011112 → 00000000	4320.000	0.646
01111002 → 00000000	4540.000	0.184
00011001 → 00000111	1708.160	0.650
00011112 → 00000111	3009.239	19.46
01111002 → 01100001	3006.663	13.43

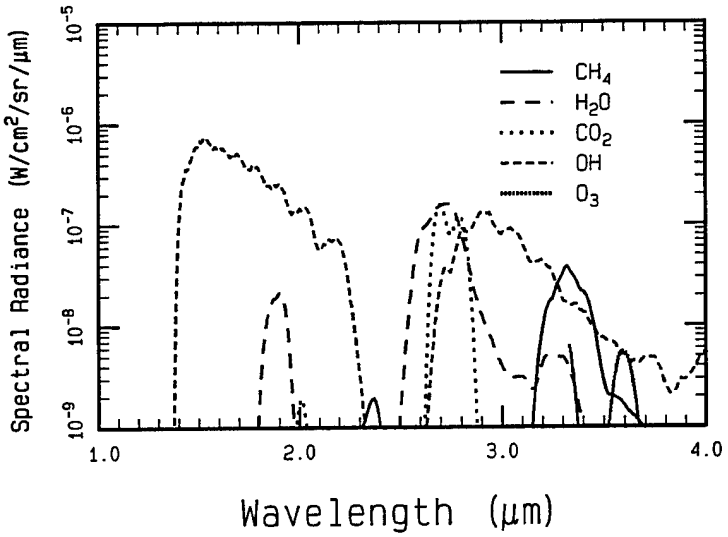

Figure 6. Contributions of Various Molecular Emitters to a Daylit 50 km Limb Calculation in the SWIR.

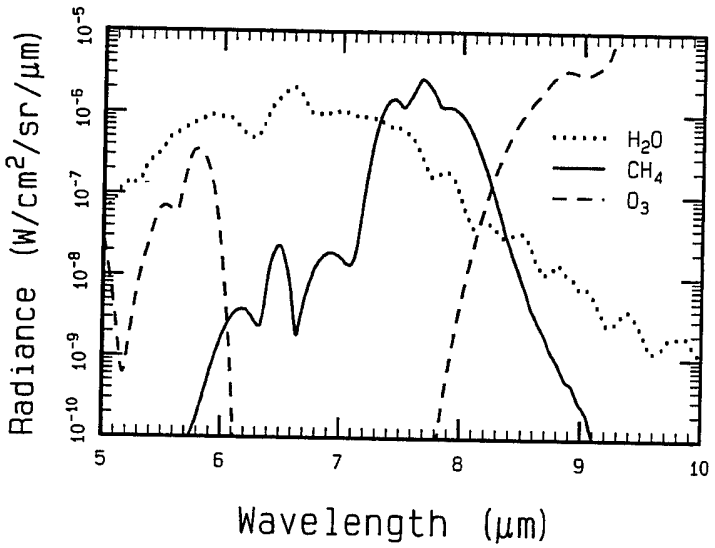

Figure 7. Contributions of Various Molecular Emitters to a Nighttime 50 km Limb Calculation in the LWIR.

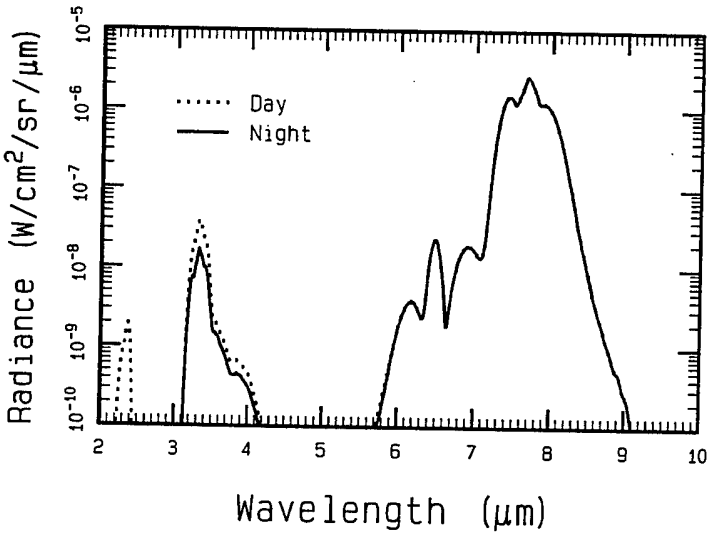

Figure 8. Effect of Solar Excitation on CH_4 Emission for a 50 km Limb.

3. OVERVIEW OF SHARC-3

SHARC calculates atmospheric radiance and transmittance under both LTE and NLTE conditions for paths above 50 km. The user has considerable latitude to modify the atmospheric model being used, both in its profile of species and in the kinetics governing the chemical and radiative processes undergone by those species. These modifications are achieved by changes to various data files, while leaving the code itself unchanged.

The spectroscopic states and bands for each radiating atmospheric species and the differential equations representing the kinetic scheme governing the NLTE energy level populations are defined in external data files rather than built into the code. Also defined via data files are the vertical concentration profiles of all atmospheric constituents, including those, such as N_2 and O, which do not contribute directly to the IR radiation but serve as collision partners in the kinetic schemes. Specific local atmospheric environments can be specified through region definitions. Diurnal characteristics within a region can be specified through multiple vertical concentration profiles which can be supplied by the user or generated for specific geomagnetic conditions by SAG, the SHARC Atmospheric Generator.[22]

For calculations involving the solar terminator, the attenuation of solar irradiance from sunlight traversing the atmosphere below 50 km, the minimum altitude treated by SHARC, must be estimated. For each radiating species, absorption parameters for the lower atmosphere have been calculated with MODTRAN and are stored in a file.

Finally, for the LOS calculation of radiation transport once the NLTE populations have been determined, spectral parameters for all individual radiating lines are tabulated in a data file.

The files, which define the species' spectroscopic states and bands and the lower-atmosphere filtering, are written in a simple ASCII format and read directly by SHARC. The kinetics scheme for a particular radiator is also written in an ASCII format, but it must be translated into a form accessible to the CHEMKIN-derived[6] AMBIENT module using it. The ASCII representation of the kinetic differential equations closely follows the notation used by chemical kineticists for publications or calculations on paper; explicit FORTRAN statements do not appear. The translation is accomplished by a separate, auxiliary program called the INTERPRETER. This program, discussed in more detail in Section 7, reads the ASCII kinetics file and produces a binary "linking" file which provides the required information for the AMBIENT module.

There are two different modes for running SHARC; they are

- interactive with input menus, or
- batch submission with a previously completed input file.

After interactively preparing the input file, the user has the option to proceed directly to execution or to exit and restart the code interactively or as a batch run. Both methods provide SHARC with an input stating the exact calculation to be performed with the information in the data files.

In the first mode, the user can specify his problem by starting SHARC in its interactive mode. All input requirements are presented to the user through a series of menus. All input is checked for consistency during the interactive session, and at the end of the session a new SHARC.INP file is created containing the verified inputs.

The SHARC interactive input module presents the user with a sequence of menus for processing SHARC.INP input files. The SHARC.INP file contains the calculation specific information. Separate menus allow the user to define the atmospheric regions which may be encountered by a LOS, in terms of atmospheric profiles, solar angles, molecular radiators, local region geometry, local ambient and auroral environments. Additional menus allow the user to select specific LOS geometries, spectral intervals and resolution. The interactive input module provides additional menus for input file name and directory selections. All inputs are checked by the program for validity and consistency so that run time errors can be minimized. Detected errors and inconsistencies are reported to the user during the interactive session so that the inputs can be repaired during the session. The existence of user selected directories and input files is also verified during the interactive session.

The second mode for running SHARC is batch submission with a previously created SHARC.INP file. In batch mode the SHARC.INP files are read by SHARC and checked for errors and inconsistencies before calculations are performed. If input errors or inconsistencies are detected the problems are reported in the SHARC.LOG file and execution is terminated before calculations are initiated.

3.1 Calculational Flow

The first step in running SHARC-3 is to insure that all needed files are available. If the program is being used as shipped, the user only needs to generate the binary linking files, generate the binary file of spectral lines, create accessible directories, and place the data files in them. One new feature of SHARC-3 is that these files no longer need to be placed in the same directory as the executable

"sharc.exe" program; during problem definition the user can specify separate directories for the various files, as outlined in more detail in Section 4 below. In SHARC-2, this capability existed only for the lines file. If modifications to the kinetics, states, bands, or atmospheric profile files are required, the user must take care to insure that the files for each radiator remain mutually consistent, as discussed in Section 7. Changes in the kinetics scheme require running the INTERPRETER program to generate the binary linking file for SHARC.

SHARC is organized into six major modules. The schematic shown in Figure 9 illustrates the calculational sequence.

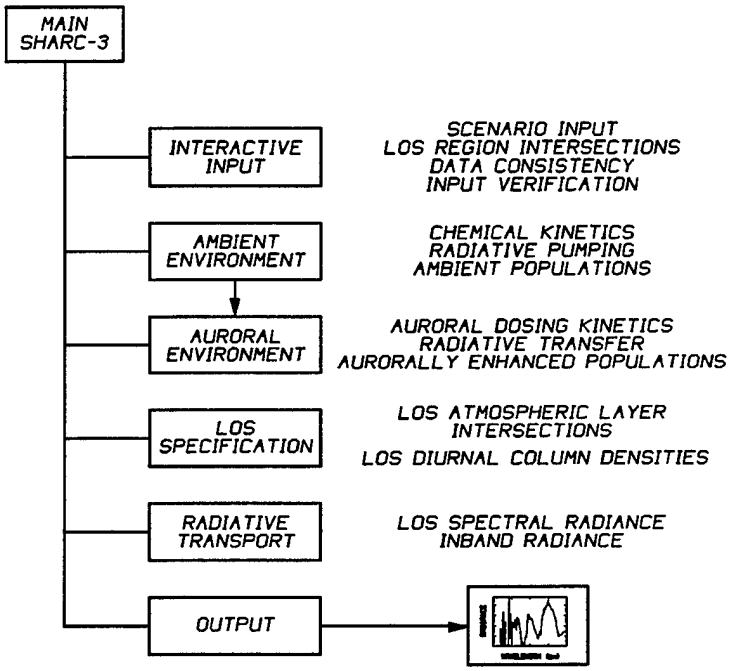

Figure 9. Calculational Sequence for SHARC.

The main module acts as a driver. First it calls the interactive module to get and verify problem specific inputs, then it calls the remaining modules to carry out the calculations and store the results.

In addition to input and verification, the interactive input module has a setup menu which allows the user to customize the installation to a computer environment.

The ambient module calculates the various molecular state populations for every atmosphere specified by the user. Each region has from one to seven atmospheres. If an auroral calculation is requested, the auroral module then calculates population enhancements for those regions designated as auroral. The LOS specification module and the radiation transport module then determine the LOS and the atmospheric radiance and transmission expected to be observed along that LOS, and the results are output for later examination.

The ambient atmospheric chemistry module calculates altitude population profiles for the various molecular vibrational states. These calculations can be lengthy, and it must be emphasized that these profiles should be re-used when different LOS paths are being calculated for the same atmospheric conditions. The ambient chemistry module includes two components, a chemical kinetics module (CHEMKIN) and a radiative transfer module (NEMESIS). Together they calculate the NLTE populations for the various molecular excited and ground states. CHEMKIN calculates excitation due to chemical reactions, energy transfer processes, and solar and earthshine pumping. NEMESIS then calculates changes in the excited-state populations due to radiative transfer between molecules in the entire atmosphere. The auroral chemistry module then calculates the auroral enhancement of these ambient populations. This module uses a time-dependent chemical kinetics module (CHEMKIN) and a simplified radiative transfer model based on Kumer's Q_w approximation to calculate the radiative transfer within the aurora.[23]

The LOS specification module divides the LOS into small segments with constant properties. For each segment it determines the local atmospheric temperature, pressure, and the molecular state column densities of each excited state. The density profiles calculated by the ambient and auroral modules are used to determine these LOS column densities.

The radiation transport module utilizes the information provided by the LOS specification module along with a molecular spectroscopic data base to determine the LOS spectral radiance. It uses an equivalent width, LBL approach in that the total path radiance from each spectral line using a Voigt lineshape is calculated. These line radiances are then accumulated in square bins, whose spectral width is defined by the spectral increment of the calculation.

3.2 Principal Modules and Features of SHARC-3

3.2.1 MAIN Module

The SHARC-3 MAIN module has a brief main program which simply passes the name of the input file, SHARC.INP, to an extensive first-level routine which carries out necessary sequence of major module calls, required to perform the tasks specified in the input.

Usually the user will place an input file (SHARC.INP), set for interactive execution, in the same directory as SHARC. The numeral "1" in the first non-comment input line specifies interactive operation. The numeral "0" in the first non-comment input line specifies batch operation. If no SHARC.INP file

exists in the same directory, a default interactive-mode file for test case 1 is created by SHARC, and an interactive session is initiated.

3.2.2 INTERACTIVE INPUT Module

When started, SHARC-3 calls the input module first, regardless of whether the mode is interactive or batch. If the SHARC.INP file is marked as interactive, the module will let the user create a new SHARC.INP file. The user defines parameters by making choices from a tree-structured series of menus; menu choices include either parameter definitions or lower-level menus. Initial parameter settings are determined by the current SHARC.INP file, which is read in before the first menu is presented to the user. The menu structure is discussed in more detail in Subsection 4.2 below. Again, the fundamental aspects of atmospheric structure and chemistry are defined in the external data files; the INPUT parameters then tell SHARC what calculation is to be performed. The user selects ambient and auroral regions, LOS specifics, molecular radiators, spectral intervals, and spectral resolution. The module also allows the user to customize the code for a particular computing environment through selection of directories for various input/output files and naming conventions for kinetics input files.

After the user has completed the inputs for the calculation, execution can be continued from the main menu. However, the more common choice is to exit the interactive session and have SHARC write a SHARC.INP that has been set for batch execution (numeral "0" in the first non-comment line).

In either mode, the code will execute, write its several output files, and stop with no further input from the user.

The LOS inputs allow arbitrary paths between 50 and 300 km. There are three general categories of LOS's supported by SHARC:

- observer to a specified source location
- observer to space
- limb viewing (space to space)

The user also has various options within these categories. The input module computes a uniform set of path quantities from the user's parameter set. Parameters for these options are discussed in Subsection 4.3.3 below. A curved-earth geometry is used for all LOS path calculations. Since atmospheric refraction is insignificant under these rarefied conditions, it is not calculated. See Subsection 4.3.4 for further details.

In addition to accepting input interactively, all intersections of the input LOS with atmospheric regions and solar zenith variations along the LOS are determined. This allows the user to assess the appropriateness of the LOS selection prior to program execution. All inputs are checked for consistency and for being within the bounds set by the program. All specified input and output files and directories are checked for their existence, status (new or old) and accessibility. All inconsistencies and file specification errors are reported to the user prior to exiting the interactive mode so that repairs can be made during the interactive session. When the batch option has been selected the input file SHARC.INP is read and this module performs all checks for input consistency and file specification errors. If inconsistencies or errors are found, an explanation of the inconsistency is written to the SHARC.LOG file, and execution is terminated.

3.2.3 Terminator and Multiple Profile Features of SHARC-3

Many properties of the atmosphere change diurnally with rapid changes occurring near dawn and dusk. The solar illumination in the atmosphere strongly influences the chemical kinetics which affects the atmospheric molecular ground and excited state populations.

A principal new feature in SHARC-3 is the ability to model these changes. Atmospheric profiles for specific latitudes and solar angles can be generated by SAG, the SHARC Atmospheric Generator. The solar pumping of excited vibrational states for any specified solar zenith angle is handled by the chemical kinetics module. A solar zenith angle grid of atmospheric profiles and excited state populations can be generated for each atmospheric region.

SHARC-3 allows the user to model the diurnal variations by selecting a set of atmospheric profiles for each atmospheric region. Each profile is associated, via menu choices made in the interactive input module, with a particular solar zenith angle of illumination. The AMBIENT module uses the solar zenith angle in its calculations of the solar pumping contributions to the excited state populations of the profile. The resulting calculations provide a set of NLTE populations at fixed solar zenith angles.

Local populations for each LOS segment are computed from this set. The altitude and local solar zenith angle of the segment are determined and the populations at that altitude are computed by interpolation.

Ideally the user will supply a set of atmospheres which evenly span the range of terminator solar zenith angles over which the species of interest undergo most of their variation. SHARC-3 copes with partial coverage using an approach based on the known structure of the terminator. If only one profile and solar zenith is supplied, populations stemming from just that profile are available for the LOS, and

the solar zenith angle is the single one specified by the user. If one day and one night profile are supplied, the day profile is used for zenith angles below a certain minimum (currently 88°) and the night profile for angles above a certain maximum (currently 102°); the terminator region between those points is treated by simple linear interpolation. As more atmospheres are included, the finer mesh for the interpolations better represents the continuous structure of the terminator. Presently each region may have up to seven profiles; this limit is set in the INCLUDE file "PARMS.H" and the minimum and maximum terminator angles are set in the routine ZNFDGE.

Preparation of the atmospheric profiles corresponding to particular solar angles in the terminator is made easier by an auxiliary program, the SHARC Atmosphere Generator (SAG),[22] discussed in Subsection 7.3 below.

3.2.3.1 Solar Angles for SHARC-3 Inputs and Calculations

Solar angles enter into specification of LOS trajectories, selection of atmospheric profiles and the contributions to solar pumping. The user must be aware of the use of all three.

In the interactive input module, the solar zenith and azimuth angles of the observer, source, tangent and intersection points with local regions are computed when the absolute LOS specification is input. The solar azimuth angles are defined as the sun-pole-(LOS point) angle. There is a relative LOS specification in which the user can specify a combination of solar zeniths and azimuths for the observer, source or tangent points. This option allows the user to directly control the change in solar zenith along the LOS.

The atmospheric profile generator, SAG, accepts solar zenith input directly or computes it from other input options. The output profile is the generator's best estimate of the vertical concentrations of atmosphere species at a given latitude, longitude, solar zenith, and time of year.

The solar contribution to radiative pumping depends on the solar zenith angle. As in previous versions of SHARC, this parameter is input independently of the atmospheric profile.

3.2.4 The Ambient Population Module

This module has two components, CHEMKIN and NEMESIS. CHEMKIN calculates excited state populations within each layer, while NEMESIS calculates the radiative interaction between states in different layers. The calculation is an iterative process; CHEMKIN starts, NEMESIS radiatively modifies some populations, and then CHEMKIN recalculates the state populations. The first component, CHEMKIN, computes the steady-state number densities of vibrationally excited atmospheric species from

a set of chemical kinetics/reaction mechanisms for each atmospheric layer. Its subroutines are based on those in the Sandia Livermore CHEMKIN package.[6]

The SHARC CHEMKIN module computes the steady-state number densities of vibrationally excited atmospheric species from the set of chemical kinetics/reaction mechanisms prepared by the INTERPRETER. The chemical kinetics equations are solved for the particular atmospheric conditions selected by the user. It calculates the formation of molecules and excited states resulting from collisional processes and the absorption of solar and/or earthshine radiation. Although the code sets up the time-dependent differential rate equations, only the steady-state solution is currently used in obtaining the vibrational state populations.

The second component in the ambient population module is NEMESIS[7] (Non-Equilibrium Molecular Emission and Scattering Intensity Subroutine) which computes the enhancement of the atmospheric excited state layer populations due to layer radiative self-trapping and layer-layer radiative pumping. Some molecular bands, in particular the 4.3 μm CO_2 band, are optically opaque to emitted radiation. Photons emitted in these bands may be absorbed and emitted many times before either escaping the atmosphere or being collisionally quenched.

The overall approach for determining the enhanced excited-state level populations involves:

- determination of the steady-state layer source populations which includes excitation by external light sources, sun and earthshine, and molecular collisions, and de-excitation by radiative decay and collisional quenching (CHEMKIN);
- determination of the first-order layer-layer population enhancement using a Monte Carlo simulation of the initial source photon emissions and their subsequent absorption or escape; and
- determination of the total enhanced populations using a recursive orders-of-enhancement approximation which is initialized by the Monte Carlo first-order results.

The source populations include all excitation sources except the internal atmospheric radiative effects of layer self-trapping and layer-layer pumping. The key results from the Monte Carlo simulation are the first-order enhancements and the probabilities that a photon emitted from a layer "i" will create a new excited state in a layer "j". This simulation involves sampling over the initial emission position, emission direction, emission frequency, emission line strength, and length of travel. The contribution of each succeeding order-of-enhancement is determined recursively by

$$(P_k) = (P_{k-1})\,(W) \quad , \tag{7}$$

where $(\mathbf{P}_k)$ is the kth-order layer population enhancement matrix, and $(\mathbf{W})$ is the layer-layer absorption probability matrix. Both $(\mathbf{P}_1)$ and $(\mathbf{W})$ are determined by the first-order Monte Carlo calculation.

The end result of each NEMESIS calculation is the total excited-state population distribution for a pair of vibrational levels, where the lower level of each pair may itself be an excited level. A cycling procedure between CHEMKIN and NEMESIS is used to step up the vibrational energy ladder until the top of the ladder is reached.

3.2.5 The AURORA Population Module

The AURORA module calculates the change in the populations of CO_2, NO and NO+ due to electron bombardment during an auroral storm. Default parameters for selecting several different strength auroras are contained in SHARC, although the user can easily define an aurora. The module performs a time dependent calculation to determine these species number densities as a function of altitude. The Gear method for stiff differential equations is used to numerically integrate the chemical kinetic rate equations describing auroral chemical and energy transfer processes. This integration package is supplied as part of the Sandia CHEMKIN code,[6] and thus it has been extensively applied to and validated against many different types of scientific problems.

In addition to the normal SHARC inputs, the following inputs are required for the AURORA module:

- definition of the strength and duration of the aurora,
- specification of the chemical kinetics mechanism for the selected radiator, including primary and secondary electron processes.

The primary electron deposition model used in SHARC is based upon the work of Grun, Rees, and Strickland and has been discussed in some detail in the AARC manual.[15] The SHARC routines describing the energy deposition have been derived from those used in AARC. The ion pair production rate is then obtained from the energy deposition rate by assuming that 35 eV are required to produce an ion pair.

The chemical reactions and energy transfer processes resulting from electron deposition in the atmosphere are also described in the AARC manual. Chemical kinetics mechanisms for NO, NO^+, and CO_2(4.3 μm) are supplied as part of the SHARC data base. The mechanisms include kinetic processes for ionization, electronic and vibrational excitation, recombination, chemical reactions, and formation of the secondary electron energy distribution. When the code exits from the auroral module, the aurorally enhanced populations are stored in an array for vibrationally excited species.

3.2.6 LOS Specification Module

The LOS specification module breaks the LOS into small segments and determines the composition and properties of each segment. The segments are determined by the intersections of the LOS with the altitude layer boundaries, defined in the input atmospheric profiles. For each segment the region and solar zenith is found and the appropriate profiles, temperatures, pressures and molecular state number densities are determined. A more detailed description of how this is performed is provided Subsection 4.2.4.

3.2.7 The Radiation Transport Module

SPCRAD computes the LOS spectral radiance using a finite-difference form of the radiative transfer equation.[3] The LOS properties are specified in homogeneous segments where each segment corresponds to the LOS path from the observer through a particular atmospheric layer (the well known Curtis-Godson approximation). A single-line equivalent width approximation based on the Voigt lineshape is used to determine the segment transmittances and radiances. This approach enables the spectral radiance to be calculated at a spectral resolution as high as 0.1 cm^{-1}. Since the radiation computation is explicitly based on the population difference of the upper and lower state, it is equally valid in both the NLTE and LTE regimes. Line strengths and locations are taken from a modified line file generated from the 1992 AFGL HITRAN line atlas[8] and augmented with additional lines as outlined in Subsection 2.3. The major modification to the line parameter database was to decompose the energy of the lower state into vibrational and rotational energies. This enables the line strengths to be scaled separately for the rotational temperature and the NLTE vibrational population of the lower level.

There is a tradeoff between speed and accuracy when dividing the atmosphere into many homogeneous layers. The LOS radiance calculation depends linearly on the number of layers. Currently the atmospheres used by SHARC are layered by 2 km steps from 50 to 150 km and by 10 km steps from 150 to 300 km. For a single region limb calculation at a tangent height of 50 km, 129 atmospheric layers are traversed by the LOS.

3.2.8 SHARC OUTPUT

The SHARC modules writes data and informational statements to four user-readable ASCII data files. The files are the journal file which is called "SHARC.LOG", the general output file, the spectral radiance

file, and transmittance file. In addition, for each profile of each region there is a binary population file, whose name is specified by the user.

SHARC.LOG contains various statements generated during a SHARC calculation. If SHARC recognizes a fatal problem, an error message is written to this file, and execution stops. A warning or caution is not fatal to SHARC, but it may alert the user that only a partial calculation has been performed or that numerical difficulties have been encountered and fixed in some module. The user should get in the habit of looking at this file after every SHARC execution to insure that the full desired calculation was actually performed. In previous releases of SHARC, this file was called SHARC.ERR. During interactive input, the user has the option of specifying that caution and warning messages, which do not stop execution, be "suppressed," i.e., not printed to the file.

The output file contains a summary of the output from each module. Three levels of output are available for each SHARC module. The level of output is selected through the interactive menu and can be defined independently of other modules. The first level contains a minimum amount of information. For example, the minimum information on the model atmosphere is simply its name. The next level of output provides more detailed information such as the number densities of the atmospheric species as a function of altitude, or the vibrational temperatures from the chemical kinetics module. Finally, the highest level of output provides intermediate results from within modules. This level of information may be necessary for "debugging" a problem encountered in SHARC, but it is usually too detailed for day-to-day execution.

The spectral and transmission files contain the spectral radiance and transmittance as a function of frequency. The resolution and frequency range are defined through the "SHARC.INP" file. The frequency unit is cm^{-1}, the radiance unit is $W/sr/cm^2/cm^{-1}$. This format is convenient for either plotting the calculated spectral radiance directly or for reducing these data further. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used in SHARC. These manipulations can be performed using the "DEGRAD" program (see Subsection 7.4).

The population file saves the excited state populations and other necessary information so multiple SHARC calculations can be performed without re-calculating the populations each time. There are two types of population files, ambient and auroral. The two types of population files have different formats, so they can be used only with the proper environment type. Populations calculated from a model atmosphere will change only when either a new model atmosphere is used, day and night conditions change, a new solar zenith angle is defined, or auroral parameters are changed. By saving and re-using these population files, a user can build up a library of population files for simulations of interest. Since

calculating the populations requires roughly half the time for a SHARC run over the full 1-40 μm spectral region, considerable time can be saved by using old population files. Population files can be reused for multiply LOS traversing the same atmospheric regions, and for different spectral intervals. The interactive input module will warn the user if an attempt is made to modify parameters which effect populations, when an old population file is in use. These warnings become errors if the code is run in batch mode. The errors are detected prior to computation. Messages describing the errors are written in the SHARC.LOG file.

4. RUNNING SHARC

4.1 Overview

This section serves as a reference for the user who wants to get SHARC-3 running without making modifications to the kinetics supplied with the code. The required files and auxiliary programs are discussed, allowing preparation of the first run. The menu system used by the INPUT module to communicate with the user is outlined in some detail. This is followed by discussions of some of the more important parameters entered through the menus. The user should read Section 3 through the end of Subsection 3.1 before reading this section. If modifications to the kinetics files are required, the user should first read Sections 6 and 7 below.

Prior to any SHARC calculation, the "linking" and "lines" files must be created. The linking files are created by running the INTERPRETER once for each radiator. The procedure is discussed in Section 7; the results will be a binary linking file for each radiator. As discussed below, these files and their associated states and bands files need not be in the same directory as the executable version of SHARC; rather, they can be placed in a separate "kinetics" directory for convenience. The spectral lines file is supplied in ASCII form as SHARC.ASC. Conversion to the binary form used by SHARC is carried out by a short program, binary.f, which the user must compile and run.

Once the user has prepared the above files, SHARC can be executed. It can be run in either an interactive or batch/background mode. The interactive mode is useful in setting up new calculational scenarios, since it walks the user through the necessary input variables. For more experienced users, SHARC can be executed by circumventing the input module and directly entering changes to the SHARC.INP file with an editor.

After a successful SHARC calculation there will be four or more new output files. These files are:

- Journal file (described in Subsection 5.1),
- General output file (described in Subsection 5.2),
- Population files (described in Subsection 5.3),
- Spectral radiance file (described in Subsection 5.4), and
- Transmittance file (described in Subsection 5.5).

The journal file, called SHARC.LOG, should be empty if the calculation was performed without errors or warnings. The user should always check this file to insure the calculation was performed correctly. The general output file summarizes the calculation. The transmittance file contains two columns giving the LOS transmission as a function of frequency (cm^{-1}). The spectral radiance file contains the spectral radiance ($W/sr/cm^2/cm^{-1}$) as a function of frequency (cm^{-1}). The population file contains the excited-state population information so that subsequent calculations can skip the population modules and go directly to the LOS specification and spectral radiance modules. To repeat for added emphasis, populations depend only on the molecular species, model atmosphere, auroral parameters, day/night conditions, and/or solar zenith angle; therefore, the same populations can be used for many different LOS's and bandpass configurations. This can save considerable computer time, and the user should develop a library of populations for often-used scenarios.

4.2 The Interactive Input Module

The SHARC input module uses a menu-query system to walk the user through the required inputs. In general, typing a 0 will take the user up a level in the menu system, while typing a number greater than 0 allows the user to input new information or enter a submenu. When a submenu is entered, current values of the input variables are displayed. This allows the user to scan the current values and decide if anything needs to be changed. The precise sequence of menus depends on choices made by the user and cannot be presented in any compact listing. Here, only the major menus will be discussed.

At the start of an interactive run, the top-level menu appears:

```
STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-3

REVIEW OR MODIFY INPUT PARAMETERS

 1) TITLE FOR CALCULATION
 2) REGION DEFINITION
 3) LOS GEOMETRY
 4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
 5) OUTPUT DATA
 6) STANDARD SET-UP FOR FILE NAMES

 7) INSTALLATION SETUP

 8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
 9) UPDATE DEFAULT FILE AND EXIT
10) EXIT WITH NO UPDATE OF DEFAULT FILE

ENTER # OF ITEM TO BE CHANGED OR
999 TO CONTINUE SHARC EXECUTION
```

Stating from the bottom, the last entries govern further execution of SHARC. An "8" exits SHARC, saving any changes that may have been made to the SHARC.INP file; a parameter is set so that the next time SHARC is run it will be in the "batch" mode, skipping the interactive session. Exiting with a "9" saves the changes but prepares for an interactive run next time. If the user wants to start over with the original input file, a "10" exits without saving any changes, and SHARC will next start in interactive mode.

Choice 7 is new to SHARC-3 and should be entered first. Previous versions required that all data files except the lines file be located in the same directory as the executable. When several users shared one computer, this feature forced duplication of common information. This new menu allows the user to specify directory paths for the data files. Also, file name patterns are set here, which eases the task of specifying file names in other parts of the menu tree. A sample menu 7 appears below. All directory and file name examples shown in this manual conform to UNIX name conventions. The directory and file names entered by the user are concatenated and stored in string variables used in the "OPEN" statements for those files. This scheme will work for non-UNIX systems if the user employs name conventions appropriate to those systems.

```
7) REVIEW OR MODIFY SET-UP STRUCTURES
 1. DIRECTORY PATH FOR THE CHEMICAL KINETICS FILES
            kindir/
 2. PREFIXES AND SUFFIXES FOR LINKING FILES
       AMBIENT  (FORMULA).LNK        AURORAL  A(FORMULA).LNK
 3. PREFIXES AND SUFFIXES FOR STATES  FILES
        AMBIENT  (FORMULA).STA       AURORAL  A(FORMULA).STA
 4. PREFIXES AND SUFFIXES FOR BANDS  FILES
          AMBIENT  (FORMULA).BND
 5. CASE SELECTION FOR KINETICS FILES    UPPER
 6. DIRECTORY PATH FOR THE PROFILES
            atmdir/
 7. CASE SELECTION FOR PROFILES          UPPER
 8. DIRECTORY PATH FOR THE POPULATIONS
            popdir/
 9. CASE SELECTION POPULATION FILES     UPPER
10. SUPPRESSION OF RUN TIME WARNINGS  NOSUPPRESSION
11. DIRECTORY PATH FOR THE LINES FILE
            lines/
12. LINES FILE NAME                    SHARC.H92
ENTER  # OF ITEM TO BE CHANGED OR
     0 TO CONTINUE
```

The user may specify different paths to various file groups. Menu item "1", specifies the path name to the kinetics (states, bands, binary linking and lower altitude transmittance Curtis-Godson) files. The file naming convention is fixed as (molecular formula).CGD. For example, for OH, the Curtis-Godson file name is OH.CGD. In menu item "6" the path name to the atmospheric profiles, in menu item "8" the path name to the population files, and in menu item "11" the path name to the lines file can be specified.

When data files are sought by SHARC, the full file names will be formed by appending the species file name to the directory name. Thus, the directory name for UNIX systems must always end in a "/", so that the full path name will be correct. For DOS systems the directory name must end in a back slash "\". To maintain compatibility with all operating systems, SHARC does not supply the "/" or the "\" when missing. The users must supply the appropriate delimiter when entering the directory name. If new population files are being generated, they will be placed in the directory specified. Items 2 through 5 and 7 specify the pattern a species or atmosphere file name will follow. When Item 2 is chosen, for example, the user will be prompted for prefixes and suffixes which will be attached to the species' name. Each species name is simply its chemical formula with the

exception of ions where a "P" is used for plus and a "M" for minus charge. For example for NO^+, the species' name in file names is NOP. This conforms with MS-DOS restrictions on use of special characters in file names.

If a new species is requested while the user is defining a region, these prefixes and suffixes will automatically be attached to create the proper file name. Null strings are acceptable, and case is determined by Items 5 and 7. Note that a change here will only affect newly chosen file names; names previously determined will not be changed unless the user goes to Item 2 of the top-level menu and makes the change. The only specific file name determined here is that of the lines file, which contains information for all species.

The first item "1", in the top-level menu permits setting the title of the calculation, which appears in the output file. The second item defines the atmospheric regions and leads to the most extensive set of sub-menus. The second-level menu of this set lists by number the regions already defined and permits definition of new ones. An example appears below.

```
2) REVIEW OR MODIFY REGION DEFINITIONS

 CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

 1. EXTENDED REGION IS AMBIENT WITH  7 PROFILE(S)

 ENTER # OF REGION TO REVIEW OR MODIFY OR
     -# TO DELETE REGION OR
      2 TO ADD REGION OR
      0 TO CONTINUE
```

Only one region has been defined thus far; this menu only tells the user that Region 1 uses 7 profiles. Typing "1" selects Region 1 for inspection:

```
   REGION DEFINITION DATA FOR REGION # 1

  1- REGION IS AMBIENT WITH   7 PROFILE(S)
  2- SOLAR ZENITH ANGLES   LOWER ATMOSPHERE AEROSOL NUMBERS
  3- MODEL ATMOSPHERE FILE NAMES
    FOR  SOLAR ZENITH  =    100.88   T4Z101.ATM
    FOR  SOLAR ZENITH  =    101.68   T4Z102.ATM
    FOR  SOLAR ZENITH  =     98.65   T4Z99.ATM
    FOR  SOLAR ZENITH  =     97.01   T4Z97.ATM
    FOR  SOLAR ZENITH  =     95.27   T4Z95.ATM
    FOR  SOLAR ZENITH  =     93.06   T4Z93.ATM
    FOR  SOLAR ZENITH  =     90.85   T4Z91.ATM
  4- CURRENT POPULATION FILE NAMES
  5- MONTE CARLO RADIATION TRANSPORT INPUTS
  6- MOLECULAR RADIATORS FOR POPULATION CALCULATION
     AMBIENT: O3
ENTER # OF ITEM TO CHANGE OR
    0 TO CONTINUE
```

In this third-level menu, Item 1 allows setting the type of the region (ambient or auroral; Region 1 must always be ambient) and the number of profiles. Each profile must have an associated file name for its defining atmosphere file, a solar zenith angle for the solar pumping calculation, and a lower-atmosphere (below 50 km) aerosol index. The aerosol index influences the absorbing effect of the lower atmosphere on sunlight when the sun is below the horizontal, as discussed more fully in Subsection 6.4. The zenith angles and aerosol indices are set under Item 2. The association of angles with file names is made under Item 3; the current angles and file names are shown in the example above. The number of files and angles can also be reduced; choosing "1" and entering a number less than 7 would truncate the list of atmospheric profile file names appearing under Item 3. In this example, the file names incorporate the values of their respective solar zenith angles; this correspondence is not required but is recommended. The T4 prefix refers to Test Case 4.

Item 4 permits the user to specify the names of the binary population files which store the results of the CHEMKIN/NEMESIS calculation. One population file is created for each atmospheric profile. The user can determine that preexisting population files be used for any of the profiles; in this case SHARC omits the CHEMKIN/NEMESIS step, saving much time. If new population data are to be calculated but not saved, scratch file names can be given for population files later discarded. A sample menu brought up by Item 4 follows:

```
     POPULATION FILE NAME(S) AND STATUS
PROFILE #  1
NEW AMBIENT                    T4Z102.POP
PROFILE #  2
NEW AMBIENT                    T4Z101.POP
PROFILE #  3
NEW AMBIENT                    T4Z99.POP
PROFILE #  4
NEW AMBIENT                    T4Z97.POP
PROFILE #  5
NEW AMBIENT                    T4Z95.POP
PROFILE #  6
NEW AMBIENT                    T4Z93.POP
PROFILE #  7
NEW AMBIENT                    T4Z91.POP
 ENTER PROFILE # OF THE POPULATION FILE(S) TO BE DEFINED OR
          0 TO CONTINUE
```

Initially an auroral region would have one OLD ambient population file and a NEW auroral file for each profile in the region.

Item 5 in the region definition menu permits setting several parameters for the NEMESIS Monte Carlo calculation. The number of trial photons and the maximum order of scattering determine the statistical error of the calculation. The user also specifies in this menu whether the SHARC calculation will use earthshine or not. See Subsection 4.3.1.

The radiators for the CHEMKIN/NEMESIS calculation are identified in Item 6. Choosing this item results in a display of radiators currently selected and the opportunity to modify or review them. In the following example, ozone is the only radiator selected.

```
   AMBIENT RADIATORS ARE:
         O3   ISOTOPE 16O

ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
   - MOLECULAR FORMULA TO REMOVE SPECIES
   0 TO CONTINUE
```

If the user enters the molecular formula, "O3", the names of the present data files for that species are displayed, and the opportunity to modify them is presented:

```
 REVIEW OF O3   INPUT DATA
 AMBIENT DATA
#  ISOTOPE     LINKING      STATES       BANDS
1   16O    O3.LLL        O3.SSS        O3.BBB


ENTER # OF ITEM TO CHANGE OR
   0 TO CONTINUE
```

Typing "1" would allow the user to modify the file names. Had the user instead entered a new formula, the program would have confirmed the species to be entered, and file names would have been constructed according to the patterns set in the second-level menu 7 discussed above. These would have been displayed to the user in the manner shown above. The user would again have the opportunity to modify the radiators. Had the user named a species for which more than one isotope is supported, the program would have detoured through a series of menus requesting specification of which isotopes were wanted before reaching the file name review menu. In this case, each isotope would have its own line in that menu, allowing independent review of each set of file names. The review step, if chosen, also displays the relative abundance of each isotope, the fraction of all molecules of a species which have that particular isotopic composition. For molecules where the separate isotopes are not distinguished in this release, the abundance equals 1.00. For the first isotope of CO_2, in contrast, the abundance equals 0.984.

Note that the O_3 file names above do not correspond to the pattern set down previously in the installation setup menu, Item 7 of the top-level menu. That pattern would have led to the names O3.LNK, O3.STA, and O3.BND. The actual file names differ either because they were entered under a different, earlier set of name patterns, or because they were created by directly editing the input file. This difference emphasizes the fact that setting a name pattern in the setup menu does not insure that these names will be used. Precedence is given to edited names; the setup names are invoked when the user adds species. The user should always check the file names. In the present menu, the switch to the *.LNK, *.STA, and *.BND patterns is most easily accomplished by removing O_3 as an included species (typing "-O3") and then adding it again (typing "O3"). The addition process will create file names with the pattern specified in the setup. If, on the other hand, O_3 is being added and the *.LLL, *.SSS, *.BBB patterns are wanted despite the setup, the user can change individual file names in the review step. The linking, states and bands files are stored along with the low altitude transmittance files in the same

directory specified in the setup. Regardless of the naming of the particular linking or states files for O_3 the O3.CGD file will be used.

In the current example, if the user backs up two levels in the menu tree (by entering "0" twice), the second-level menu will again be displayed:

```
2) REVIEW OR MODIFY REGION DEFINITIONS

 CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

1. EXTENDED REGION IS AMBIENT WITH  7 PROFILE(S)

 ENTER # OF REGION TO REVIEW OR MODIFY OR
      -# TO DELETE REGION OR
       2 TO ADD REGION OR
       0 TO CONTINUE
```

Entering "2" will bring up the region definition menu for the entirely undefined Region 2:

```
  NEW REGION PARAMETERS FOR REGION #  2
 1- REGION ENVIRONMENT AND STRUCTURE
 2- SOLAR ZENITH ANGLE   LOWER ATMOSPHERE AEROSOL NUMBER
 3- MODEL ATMOSPHERE FILE NAME
 4- INPUT NEW POPULATION FILE NAMES
 5- MONTE CARLO RADIATION TRANSPORT INPUTS
 6- MOLECULAR RADIATORS FOR POPULATION CALCULATION
 7- AURORAL MODEL PARAMETERS
 8- REGION BOUNDARIES

ENTER # OF ITEM TO INPUT DATA OR
    0 TO CONTINUE
```

The user would then proceed through the options much as before, entering the various parameters. Note that all regions after the first one are local. They may be auroral, so Items 7 and 8 for setting auroral and boundary parameters appear for the first time. The auroral parameters are discussed in Subsection 4.3.2.

The third item in the top-level menu, "LOS GEOMETRY," leads to a set of menus for setting various geometrical parameters:

```
3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

 CURRENT LOS DEFINITION:
 1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NORTH POLE
 2. SUN LOCATION
    SOLAR LATITUDE:   -1.7  LONGITUDE:   304.4 DEGREES
 3. SPHERICAL EARTH ASSUMED
 4. ABSOLUTE LOS LOCATION SPECIFICATION
    DIRECT INPUT OF LATITUDE/LONGITUDE INFORMATION
 5. PATH TYPE IS OBSERVER TO SPACE
    OBSERVER INFORMATION
    OBSERVER ALTITUDE:    183.80 KM
    OBSERVER LONGITUDE:   213.450 DEGREES
    OBSERVER LATITUDE:    65.803 DEGREES

    SOURCE INFORMATION
    TANGENT HEIGHT:     95.97 KM
    LOS FORCED THRU LONGITUDE:  198.720 DEGREES
    LOS FORCED THRU LATITUDE:   73.772 DEGREES

ENTER # OF ITEM TO CHANGE OR
     0 TO CONTINUE
```

Here, Item 1 allows the choice of either the magnetic or geographic pole as the origin of the coordinate system. The point immediately below the sun is established in Item 2; this information is used to determine solar illumination angles during the LOS calculation. In Item 3 the user chooses between a spherical or oblate spheroidal earth. Item 4 distinguishes between two methods for defining the LOS:

- by the latitude, in degrees north of the equator, and longitude, in degrees east of Greenwich, of reference points beneath the LOS (Absolute LOS specification, as shown above), or
- by the solar zenith and azimuthal angles of such reference points (sun-relative LOS specification).

After setting these parameters, the user defines the LOS path in Item 5. Three path types are allowed: observer (at some location) to a source point, observer to space (the point where a LOS reaches 300 km altitude is considered space), and limb view (from 300 km to 300 km, passing through a specified tangent height). For each path type, the user is presented with a list of options for defining the path. The options available are constrained by the path type and the earlier choice of absolute/relative LOS specification. See Subsections 4.3.3 and 4.3.4 below for diagrams showing the geometries for the several path types. These menu options provide flexibility in LOS definition. Cycling through them can enable

the user to develop a desired LOS iteratively, using the SHARC geometry package rather than calculating reference points outside the code.

The fourth top-level item specifies the spectral interval and the spectral resolution of the calculation. Also, the radiators to be included in the LOS radiation transport calculation are named. These must be a subset of the radiators treated in the population calculation; a species' contribution to radiance and transmittance cannot be determined if its various population levels have not been calculated!

Item 5 of the top-level menu determines what information will be placed in the output file. The possible options are discussed in Subsection 3.2.8 above.

The sixth top-level item allows the user to choose root names for the output, radiance and transmission files and the directory where they will be placed.

4.3 Input Parameters

This section describes key input parameters for the ambient and auroral populations, LOS geometry and radiation transport modules. The Monte Carlo control parameters used in the ambient populations module warrant further discussion since their values affect the accuracy of this stochastic simulation. Parameters used to define the auroral conditions are discussed in detail. The Geometry parameters section describes the various subsets of geometry variables needed to define an LOS. Finally the parameters used to define the spectral interval, resolution, and species included in the calculation are discussed.

4.3.1 Ambient Population Parameters

The ambient populations module contains a set of routines that determine the enhancement of the species excited-states population profiles due to layer radiative self-trapping and layer-layer radiative pumping. The first-order population enhancement is determined using a Monte Carlo simulation of the initial photon emission and its subsequent absorption or escape. The number of photons determines the statistical uncertainty of the Monte Carlo calculation. Changing this variable to a small number saves computer time, but causes large statistical uncertainties. For reasonable statistical uncertainties the number of photons should be 10,000 or larger.

The maximum order of scattering determines the number of matrix multiplications, Equation (7), used by NEMESIS to calculate the population enhancement matrix. Changing this number to less than 100 does not save much computer time since the Monte Carlo simulation is performed for first-order

scattering only and higher order scattering is determined recursively. Many orders of scattering may be important for some molecular bands, such as 4.3 μm CO_2 radiation. A value of 200 for the maximum order of scattering is sufficiently large.

The remaining parameter governs earthshine pumping. A value of 1 means the pumping is on, and a value of 0 means the pumping is off.

4.3.2 Auroral Population Parameters

The model parameters describing an auroral event allow the user to either select a code supplied aurora or to define a user specified aurora, as well as to specify the duration of the aurora and observation time. As developed in AARC,[15] two simple forms for the auroral primary electron spectral flux are available in SHARC, a Maxwellian flux and a Gaussian flux. The Maxwellian flux is representative of diffuse auroras and is characterized by two parameters, the total energy flux and a characteristic energy (equal to one half the mean energy). The Gaussian flux is characteristic of electron energy spectra in discrete auroras and is defined by three parameters, the total flux, mean energy, and variance of the incident electron energy. However, the user can select three typical auroral electron spectra with a Maxwellian distribution corresponding to IBC classes of II, III, or III$^+$. Finally, the user must select the duration of the aurora, and the observation time relative to the beginning of the dosing (which is assumed to be 0). The input units are:

- flux: ergs/cm^2/sec,
- energy: KeV, and
- time: sec.

4.3.3 Local Region Geometry

Auroral excitation is confined to a finite region within the atmosphere. SHARC-3 has separate sets of atmospheric profiles for each local region and for the rest of the atmosphere. Each local region that is auroral has its own set of auroral parameters. The auroral radiance calculation for the specified LOS can be done either during the dosing or at some period subsequent to it.

A local region is defined by four (latitude, longitude) points plus the upper and lower altitudes of the region. The four points must form a convex quadrilateral, which has no interior angles greater than 180°. A coordinate system pole cannot be within a local region. If a pole is to be within an auroral region, the input geometry should use the alternate geographic coordinate system, e.g., use coordinates centered on the geographic pole when the auroral region includes the geomagnetic pole. The altitude profile used for

the local region must be extended down to 50 km even though the lower boundary of the region is much higher. This is necessary because the NEMESIS calculation for radiative excitation requires a full profile in order to get the proper upwelling earthshine and layer to layer radiative pumping. For the LOS radiance calculations, SHARC uses the populations from the extended region below the region's lower altitude boundary and above the regions upper altitude boundary.

Usually the LOS of the radiance calculation only intersects the local region twice. A typical path is illustrated in Figure 10. However, because of earth curvature effects, four intersections are possible for a limb path whose minimum altitude is just slightly less than the lower region boundary. For example, a limb path at 89 km combined with a lower region boundary of 90 km will have four intersections when the horizontal extent of the region is several hundred kilometers to each side of the tangent point.

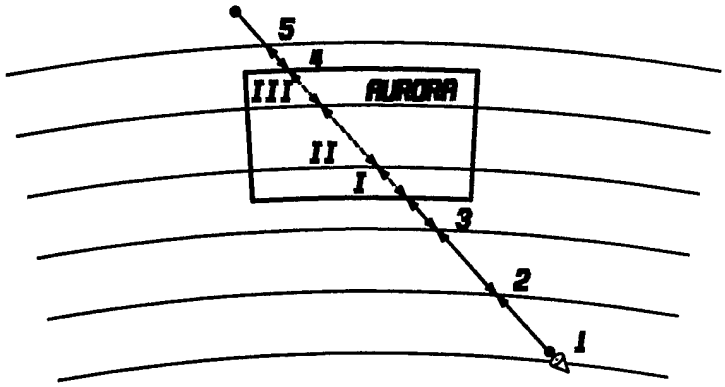

Figure 10. Layering Schematic with Local Auroral Region.

4.3.4 Line-Of-Sight Parameters

The LOS is defined as the straight line that connects the observer located at a point H_1 to the source located at H_2. Curvature of the LOS due to refraction is negligible over the altitude regime considered in SHARC. Three classes of LOS paths are supported by SHARC and are specified through a path parameter:

PATH = 2 -- observer to source,
= 3 -- observer to space, and
= 4 -- limb viewing.

The geometry nomenclature is derived from the low- altitude radiance code LOWTRAN 6.[24] In the current SHARC version, there is no PATH = 1 option. There are a number of geometric parameters that must be specified to define the LOS path, and these are defined in Table 3 and illustrated in Figures 11 and 12. Altitudes and ranges are given in km, and angles in degrees. Longitudes can have values ranging from 0° to 360° east of Greenwich, and latitudes, from -90° at the south pole to 90° at the north pole. A_0 is the local zenith angle of the LOS as measured from the vertical line connecting H_1 and the earth center. The angle B_0 is the azimuth of the LOS measured in degrees east of north from the observer; it varies from -180° to 180°.

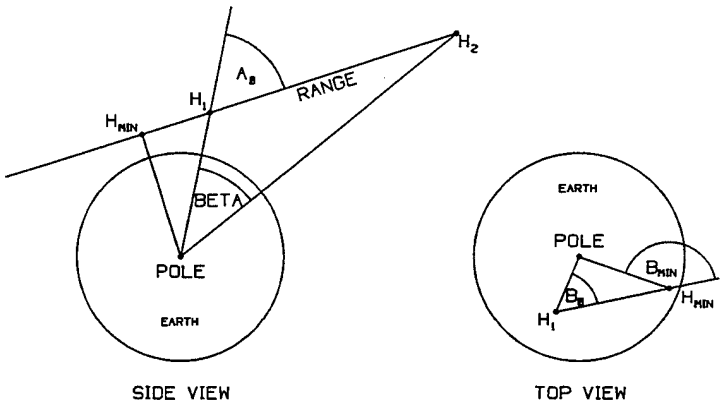

Figure 11. Definitions of LOS Angles Range and Altitudes.

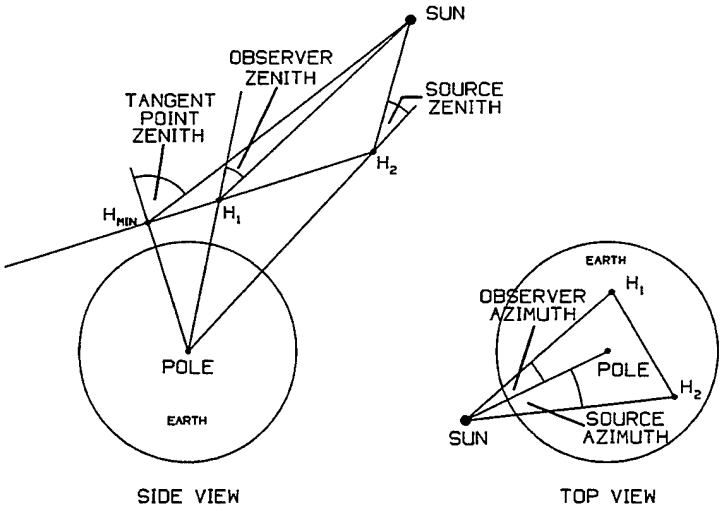

Figure 12. Definitions of LOS Solar Angles.

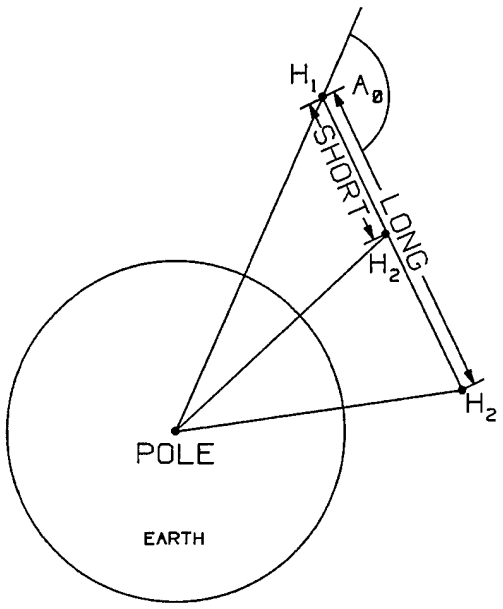

Figure 13. Illustration of Short and Long LOS Down-Looking Paths.

The parameters listed in Table 3 overspecify the LOS. For a particular LOS only one of many different subsets is required as input. The other parameters are calculated internally. Each class, designated by its PATH value, has various options for specifying the LOS. These are labeled by CASE and are listed in Table 4 along with the required geometrical inputs. The particular case with PATH = 2 and CASE = 1 can be ambiguous when observer altitude is greater than the source altitude and the LOS zenith, A_0, is greater than 90^O. This is a down looking scenario in which the source point is either before the tangent point (short) or past the tangent point (long). SHARC allows observer to space LOS for which the observer is either up looking or down looking. Thus the LOS must be specified short or long whenever using the PATH = 3 and CASE = 2 option. Two paths distinguished by LOS = (short,long) are illustrated in Figure 13.

Table 3. LOS Parameters.

SOLAR LOCATION (SUN)
- longitude
- latitude

OBSERVER POINT PARAMETERS (H_1)
- altitude
- longitude
- latitude
- solar zenith
- solar azimuth (pole-sun-observer)

SOURCE POINT PARAMETERS (H_2)
- altitude
- longitude
- latitude
- solar zenith
- solar azimuth (pole-sun-source)

TANGENT POINT PARAMETERS (H_{min})
- altitude
- longitude
- latitude
- solar zenith
- solar azimuth (pole-sun-tangent point)

ARBITRARY POINT PARAMETERS (H_p)
- longitude
- latitude
- solar zenith
- solar azimuth (pole-sun-point)

LOS LENGTH AND ORIENTATION PARAMETERS
- RANGE, the distance from observer to source, H_1 to H_2
- LOS paths which do not include the tangent point are short.
- LOS paths which do include the tangent point are long.
- BETA, the earth-center angle between H_1 and H_2
- A_0 the zenith angle of LOS at observer
- B_0, the (pole-observer-LOS) azimuthal angle;
- B_{min}, the (pole-tangent point-LOS) azimuthal angle;

Note: All azimuths defined as (north = 0^o & east = 90^o).

Table 4. Geometry Input Sequences.

PATH	CASE	Geometrical Inputs
2	1	H_1, H_2 (altitude), A_0, B_0
		H_1, H_2 (altitude), A_0, B_0, (short/long)
	2	H_1, RANGE, A_0, B_0
	3	H_1, H_2 (altitude), RANGE, B_0
	4	H_1, H_2 (altitude), BETA, B_0
	5	H_1, H_2
3	1	H_1, A_0, B_0
	2	H_1, H_{min} (altitude), B_0, (short/long)
4	1	H_{min}, B_{min}

Note:
1. There are two ways to enter the point H_1.
   H_1(altitude, latitude, longitude) or
   H_1(altitude, solar zenith, solar azimuth)
   for absolute or relative specification respectively
   H_2 and H_{min} are defined analogously.

2. there are three ways to input the observer LOS azimuth angle B_0:
   (1) direct entry in degrees,
   (2) defining a point along the LOS trajectory before H_1
   (3) defining a point along the LOS trajectory after H_1

3. there are three ways to input the tangent point azimuth angle B_{min}:
   (1) direct entry in degrees,
   (2) defining a point along the LOS trajectory before H_{min}
   (3) defining a point along the LOS trajectory after H_{min}

4.3.4.1 Forcing the LOS to Intersect Regions

One of the uses of the arbitrary point option (H_p) for specifying the LOS azimuth angles is to orient the LOS so that it intersects a particular region. If the point option is used, specifying the point latitude and longitude within local region will force the LOS to intersect the region if it passes within the upper and lower region altitude. The arbitrary point option can be used to control the change in zenith angle over a LOS. For example by using the relative option, and specifying the arbitrary point solar zenith as the same as the source (or tangent point value) the LOS would be oriented parallel to the terminator.

4.3.5 Spectral Radiance Parameters

The spectral range is defined by specifying the minimum and maximum frequency (cm^{-1}) of interest. SHARC currently includes lines from 250 to 10000 cm^{-1}. The spectral resolution is given in cm^{-1} and is currently limited to 0.1 cm^{-1}. The spectral radiance array can contain 10,000 points. So, if 0.1 resolution is used only a 1000 cm^{-1} spectral interval can be used. The interactive input module will alert the user if the interval is too large for the selected resolution and then reset the maximum frequency to reduce the interval.

The user must specify the species desired for the radiance calculation. The list may be equal to, or a subset of the species contained in population calculations or population files. The species are entered through the interactive input module by typing in their chemical formulas. At the end of a calculation the total number of spectral lines are summarized for each band and species in the general SHARC output file.

5. SHARC-3 OUTPUT FILES

5.1 Journal File

The SHARC journal file (SHARC.LOG) contains various informational statements generated during SHARC execution. The majority of messages are due to problems encountered with parameters in the input files. Warning or caution messages usually result from inconsistent use of input files. An error message during execution is considered fatal, and execution will stop after the error message is written to the journal file. A warning or caution message is not fatal (that is, does not terminate execution), but it should inform the user that input files are inconsistent, that only a partial calculation has been performed, or that numerical difficulties have been encountered and fixed in one of the SHARC modules. The user should monitor the journal file after each SHARC run to insure that the desired calculation was properly performed. During auroral calculations, several warning messages are routinely given stating that different molecular species were not found. Since auroral excitation is only calculated for CO_2, NO, and NO+, these messages are reasonable, but the user should check that these species were not inadvertently omitted too.

There are over 150 different error/caution messages that can be written during execution. These messages contain the name of the subroutine in which the problem occurred. For example, consider an error resulting from inconsistent input in the molecular states and bands files (see Subsections 6.2 and 6.3, respectively). Assume that the 2→1 vibrational transition for CO has been specified in the molecular states file (see Table 8 in Section 7). If the data for the line strength distribution function for the 2→1 transition have not been included in the molecular bands file (see Table 9 in Section 7), the following error message will be written to the journal file:

```
ERROR IN BANDIN...
    CO(2)     - CO(1)     BAND MISSING FROM BAND DATA
```

prompting the user to check the CO bands file for either an input error or omission of data.

As seen in this example, the error/caution messages generated from the input files are usually self-explanatory, and the user should be able to easily correct the problem. In some cases, however, the problem may be more subtle. For example, messages generated during calculation of number densities of vibrationally excited states most likely will require the user to carefully check the chemical kinetics mechanism and the list of transitions considered by the ambient populations module.

5.2 General Output File

The general SHARC output file contains a summary of selected output from each module. As mentioned previously, three levels of output (0,1,2) can be obtained from each SHARC module. The level (and amount) of output is selected through the interactive menu (see Subsection 3.2.8). The level of output is controlled independently for various modules. The lowest level contains the minimum amount of information (level=0) necessary to characterize the calculation, and the highest level contains the maximum amount of information (level=2). The information written to the output file for the level options is illustrated in Table 5. Notice that the atmosphere name and the band radiance summary are always written to the output file, and the spectral radiance as a function of frequency is always written to the spectral file.

5.3 Population File

For a given set of species and kinetic schemes, the excited-state populations for each atmospheric layer change only when atmospheric conditions change; some examples are a new model atmosphere, day and night conditions, new solar zenith angle, or auroral conditions. The excited-state populations and the information necessary to characterize them uniquely are written to a binary "population" file. This allows the user to perform multiple SHARC calculations for any number of observer-source scenarios without re-calculating the populations each time. The relevant information written to the "population" file is:

- Name of the model atmosphere file (Subsection 6.6),
- Names of the molecular radiators and the associated "linking", "states", and "bands" files,
- The list of species (Subsection 7.1) for each molecular radiator,
- The molecular states file (Subsection 6.2) for each molecular radiator,
- The state populations and associated temperatures for each radiator, and
- The auroral parameters when the auroral option is used.

Table 5. Type of Output Contained in SHARC.OUT File.

OUTPUT	OPTION	DESCRIPTION
Model Atmosphere	0	Atmosphere file name
	1,2	complete atmospheric input file
Selected Transitions	0	No output
	1,2	complete molecular states input file
Molecular Band Data	0,1	No output
	2	complete molecular bands input file
Ambient Output	0	No output
	1	initial steady state layer source populations and nemesis excited state population enhancements; earthshine, sunshine, and atmospheric excitation rates; and the quenching/re-emission probabilities
	2	post NEMESIS excited state populations for each selected transition
Auroral Output	0	No output
	1	final population for all auroral species
	2	populations of all auroral species as a function of time
Final Excited State Populations	0	No Output
	1,2	final excited state populations
Final Excited State Temperatures	0	No Output
	1,2	final excited state temperatures
Line of Sight Output	0	
	1,2	Species total column densities along line of sight
Spectral Radiance Output	0	Plot file (SHARC.SPC)
	1,2	spectral radiance table

For subsequent calculations with the same "population" files, it is only necessary to change the input and output parameters relevant to the LOS specification and/or radiation transport sections of the SHARC.INP file (Subsections 4.2 - 4.3). Although the complete set of options listed in Table 5 for the amount of detail in the general output file are not available when using a previously created population file, the output file does contain sufficient detail to characterize uniquely the population file used. However, the user should refer back to the original general output file generated when the population file was created if greater detail is desired.

5.4 Spectral File

An ASCII file is created to allow the user either to plot the calculated spectral radiance directly or to reduce the results further. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used by SHARC. The plot file contains two columns with the frequency (cm^{-1}) and the spectral radiance ($W/sr/cm^2/cm^{-1}$) written as an (x,y) ordered pair.

5.5 Transmittance File

An ASCII file is created to allow the user either to plot the calculated spectral transmittance directly or to reduce the data further. For example, the user may wish to apply a specific filter function to the transmittance or to convert to a set of units other than those used by SHARC. The plot file contains two columns with the frequency (cm^{-1}) and transmittance written as an (x,y) ordered pair.

6. SHARC DATA FILES

The particular species, isotopes, states, transitions, concentration profiles, and reaction schemes used by SHARC-3 to determine atmospheric radiance and transmission are not built into the code. They are specified by the user through input data files. A basic set is supplied for the SHARC radiators. A radiator is defined as a particular isotope of a chemical species (e.g. the three isotopes of CO_2, or major isotope of O_3). Four files are supplied for each radiator which together define the relevant species dependent chemistry. These are the kinetics/linking, states, bands, and low-altitude transmittance files. In addition, the vertical concentration profiles of all species at a given location are set in the model atmosphere files. The user may use these files as shipped, but may also modify the chemistry by changing the files. To permit such modifications, their structures are described below.

6.1 Kinetics Files

The populations for the various vibrational levels of the radiating species are calculated with a kinetic model using rate equations for the important processes. Each species is treated separately. As discussed above, SHARC does not have a particular kinetics model built into the software. The user specifies the important reactions for each molecular radiator through its kinetic file. This file contains a description of all the reactions in the model, written in an ASCII format as a kineticist would write them. An important auxiliary program, the INTERPRETER, reads these files and translates them into a binary linking file which is read and used by SHARC itself.

A number of considerations apply when the kinetics files are created or modified. The required information, the flexible formats and the INTERPRETER program are discussed in Subsection 7.1 below.

6.2 Molecular States Files

The molecular states files supply the following information to SHARC:

- Identification of the molecular radiator;
- Definition of the vibrational energies and degeneracies associated with the vibrational states included in the chemical kinetics mechanism;

- Definition of the vibrational transitions (that is, molecular bands) which will be treated by NEMESIS and SPCRAD. Note that a transition may be considered by NEMESIS but not by SPCRAD; and

- Definition of an effective earthshine temperature for each transition considered by NEMESIS.

The molecular states file is written in ASCII format. The information is stored in all 80 columns and is format free. The SHARC CO molecular states file is given in Table 6. As the structure of the molecular states file is described, the reader should refer back to Table 6 as an example of the file organization.

The first line in the states file identifies the radiating species (which must be the first entry on this line). Any subsequent information on this line is treated as a comment and ignored by the code. The next line must contain the identifier ENERGIES starting in Column 1 and thus signals the start of the list of vibrational-state energies and degeneracies. This line is followed by any number of lines, each of which must contain three numbers to identify the particular vibrational state (using the standard AFGL notation), the energy of that state (in cm^{-1}), and the degeneracy of that state, respectively. Numbers must be separated by at least one blank, and they may be integer, floating point or exponential. After all vibrational states have been listed, the next line must contain the word END beginning in Column 1.

The next section of the molecular states file lists information about the vibrational transitions. The first line following the END line must contain the word TRANSITIONS starting in Column 1. This line is followed by as many lines as necessary to identify: each vibrational transition considered by NEMESIS, the effective earthshine temperature (in K) for the transition, and whether or not to compute the radiance along the observer LOS for the transition. The vibrational transition is listed as "U-L" where "U" denotes the upper state and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. It is important to note that a transition in the molecular states file must have the corresponding radiative relaxation and excitation processes listed in the chemical kinetics mechanism (compare Table 13 of Section 7 below, and Table 6 above). The LOS radiance option is defined as follows:

- 0 - Radiance is <u>not</u> computed for this transition,

- 1 - Radiance is computed for this transition.

Although the radiance may not be computed for a particular transition, it may be important for the NEMESIS calculation to include the transition in the states file. Each entry, vibrational transition, effective earthshine temperature, and LOS radiance option must be separated by at least one blank. After

all the vibrational transitions information has been given, a line containing the word END beginning in Column 1 must follow.

Table 6. SHARC CO Molecular States Input File.

```
CO VIBRATIONAL STATES AND TRANSITIONS
ENERGIES AND DEGENERACIES
 0        0.000              1
 1             2143.272              1
 2        4260.063           1
END
TRANSITIONS
 1-0          230.0          1
 2-0          280.0          1
 2-1          280.0          1
END
```

6.3 Molecular Bands Files

The molecular bands files are used to input line strength information for the ambient population module. Bands files are not used in the auroral calculations. This information is used to obtain the altitude-dependent earthshine and sunshine excitation rates and to calculate the enhancement of molecular excited-state populations due to radiative trapping and atmospheric emission.

Although the ambient population module could use the modified HITRAN line compilation directly, this would be extremely time consuming due to the large number of lines. It is much more efficient to discretize the line strength distribution for each molecular vibrational state. Finite width bins are chosen in which a single average line is determined, and a degeneracy equal to the actual number of lines from the exact distribution is assigned to the average line. In the limit of infinitesimal width bins the exact line strength distribution is recovered. For reasonable choices of bin widths (presently three bins per order of magnitude), the number of lines that need be considered can be reduced by several orders of magnitude without significant loss of computational accuracy.

The molecular bands file indicates the vibrational transition along with the number of lines in a bin, and the average strength in the bin at the specified temperature. This information suffices to completely characterize the discretized line strength distribution at each temperature. The file is written in ASCII format using all 80 columns and is format free. The molecular bands file for CO is given in Table 7. Again, the reader should refer back to Table 7 as an example of the file organization.

The first line in the bands file identifies the molecular species (which must be the first entry on this line) for which the file has been created. Subsequent information on this line is treated only as a comment and is ignored by the code. The molecular species is checked against the radiating species identified in the molecular states file to ensure a consistent set of files is being used. The second line contains the vibrational transition which is then followed by a list of headings for the columns beneath; "G" indicates the number of lines, and "SBAR" means average line strength. As in the molecular states file, the vibrational transition is listed as "U-L" where "U" denotes the upper state, and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. Each transition listed in the molecular states file must have a corresponding entry in the molecular bands file. The next line notes the number of temperatures and the temperatures at which the strength distribution was calculated. The following lines describe the line strength distribution. Each line contains the number of lines in that energy bin and the average line strength at each temperature. The entries must be in the following order:

1. the number of lines in the bin,
2. the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_1,
3. the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_2 continuing up to the nth temperature.

After all the line strength bins have been listed for the particular transition, the next line must contain the word END beginning in Column 1.

Table 7. SHARC CO Molecular Bands Input File.

CO	BAND TRANSITIONS FOR ISOTOPE NUMBER 1						
	1-	0	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			23	0.375E-18	0.352E-18	0.329E-18	0.254E-18	0.149E-18
			9	0.109E-18	0.138E-18	0.161E-18	0.198E-18	0.169E-18
			5	0.324E-19	0.605E-19	0.890E-19	0.167E-18	0.189E-18
			4	0.111E-19	0.265E-19	0.459E-19	0.119E-18	0.171E-18
			4	0.387E-20	0.116E-19	0.234E-19	0.823E-19	0.149E-18
			4	0.120E-20	0.461E-20	0.110E-19	0.541E-19	0.126E-18
			4	0.330E-21	0.167E-20	0.477E-20	0.338E-19	0.104E-18
			3	0.919E-22	0.612E-21	0.210E-20	0.215E-19	0.868E-19
			3	0.326E-22	0.266E-21	0.105E-20	0.141E-19	0.699E-19
			2	0.111E-22	0.115E-21	0.532E-21	0.973E-20	0.604E-19
			4	0.349E-23	0.455E-22	0.245E-21	0.617E-20	0.491E-19
			2	0.871E-24	0.154E-22	0.101E-21	0.372E-20	0.391E-19
			2	0.353E-24	0.749E-23	0.556E-22	0.264E-20	0.334E-19
			3	0.112E-24	0.299E-23	0.259E-22	0.169E-20	0.277E-19
			5	0.205E-25	0.746E-24	0.801E-23	0.821E-21	0.191E-19
END								
	2-	0	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			22	0.294E-20	0.274E-20	0.255E-20	0.195E-20	0.118E-20
			10	0.890E-21	0.112E-20	0.130E-20	0.158E-20	0.138E-20
			5	0.245E-21	0.458E-21	0.674E-21	0.127E-20	0.151E-20
			5	0.775E-22	0.189E-21	0.333E-21	0.898E-21	0.139E-20
			4	0.225E-22	0.714E-22	0.150E-21	0.573E-21	0.116E-20
			3	0.773E-23	0.307E-22	0.745E-22	0.381E-21	0.955E-21
			4	0.257E-23	0.130E-22	0.372E-22	0.265E-21	0.847E-21
			3	0.734E-24	0.491E-23	0.169E-22	0.173E-21	0.733E-21
			3	0.240E-24	0.197E-23	0.779E-23	0.106E-21	0.552E-21
			3	0.736E-25	0.795E-24	0.377E-23	0.737E-22	0.505E-21
			2	0.254E-25	0.336E-24	0.183E-23	0.473E-22	0.400E-21
END								
	2-	1	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			22	0.755E-18	0.711E-18	0.667E-18	0.515E-18	0.303E-18
			9	0.220E-18	0.277E-18	0.322E-18	0.395E-18	0.333E-18
			6	0.635E-19	0.109E-18	0.156E-18	0.282E-18	0.314E-18
			5	0.206E-19	0.497E-19	0.867E-19	0.230E-18	0.337E-18
			3	0.714E-20	0.216E-19	0.439E-19	0.157E-18	0.286E-18
END								

6.4 Low Altitude Transmittance Curtis-Godson Files

These files are needed for solar zeniths between 90° and 108°. For angles above ≈ 108° the SHARC atmosphere is below the terminator and no solar pumping of the SHARC atmosphere is occurring. The nighttime atmosphere is appropriate and no Curtis-Godson file is required. When the solar zenith is between 90° and 108°, the atmosphere is pumped by solar radiation that has passed through parts of the atmosphere that are below SHARC's lower boundary, 50 km. Since some of this radiation is absorbed by the lower atmosphere, it cannot be represented by an unfiltered solar spectral distribution. The amount of absorption at any wavelength is determined by the solar zenith angle, or equivalently the minimum altitude through which the sunlight passes, and by the aerosol content of the lower atmosphere.

SHARC-3 models the attenuation of solar irradiance by "continuum" sources using precalculated transmittances. Here the term continuum denotes all absorbers other than the particular chemical species for which solar excitation rates are being calculated. For each vibrational band, lower atmosphere (< 50 km) continuum transmittances are stored for three aerosol profiles and five solar zenith angles, a total of 15 values. Part of the data for the ν_1 band of CO are presented in Table 8. As before, the first line identifies the molecular species. The second line identifies the vibrational transition and its frequency. The third line of the table contains the sines of the solar zenith angles at 50 km altitude. For 50 km solar zenith angles exceeding 97.029° [sin(97.029°) = .99248427], the refractive path intersects the earth. The three lines of data which follow in the table (above the word CNTEND) contain the negative logarithm of the transmissions. The pre-selected MODTRAN aerosol models are (1) no aerosol, (2) low level of aerosols [rural boundary layer with 23 km sea-level visibility and background stratospheric profiles and extinction], and (3) high level of aerosols [rural boundary layer with 5 km sea-level visibility and an extreme volcanic profile].

SHARC has always modeled the line center attenuation of solar irradiance by performing line-by-line calculations using an approximate distribution of lines from a BANDS file to describe each vibrational transition. Curtis-Godson averages are used to define Doppler and collision broadened half-widths for the solar paths. For solar zenith angles between 90° and 108°, it is necessary to determine the lower atmosphere contributions to the Curtis-Godson sums. These values are tabulated in the Curtis-Godson, *.CGD, files. For each line of a BANDS file, there are 15 entries in the *.CGD files. The entries are the optical depth (cm^{-1}), the Doppler half-width (cm^{-2}) and the collision half-width (cm^{-2}) sum for each of the five 50 km altitude solar zenith angles. In actuality, the logarithms of the sums are stored in order to expedite exponential interpolation at intermediate solar zenith angles. Table 8 contains these values for the CO ν_1 band. The first three lines following CNTEND contain the sums for the first line in the

BAND file. The next three lines correspond to the second line in the BAND file, and so on. The file names used are (molecular formula).CGD. These files must be located in the same directory as the chemical kinetics files.

Table 8. Curtis-Godson File for Part of CO (ν_1 Transition Only).

CO	BAND TRANSITIONS FOR ISOTOPE NUMBER 1				
	1- 0	2143.27 CM-1			
	5 0.99849671	0.99549103	0.99398768	0.99323565	0.99248427
	0.04301865	0.33140495	0.85715795	2.21468997	13.31810570
	0.04409396	0.34464619	0.88809311	2.26152062	17.39599419
	0.04409396	4.05797625	5.64853382	5.83024502	36.60150146
CNTEND					
	-3.2660232	-0.9006076	2.2183902	3.4376051	4.2762532
	-9.3289385	-7.0368724	-3.9300308	-2.6604104	-1.7629615
	-11.9056187	-6.7386403	-1.8185773	0.0620786	1.5002630
	-4.1675000	-1.9951240	1.0907841	2.4471624	3.4327543
	.				
	.				
	.				
	-22.8925648	-19.3326969	-14.5496349	-11.7044821	-8.4952393
	-15.4139004	-14.6549358	-11.9066591	-9.7788496	-7.0495329
	-21.4729557	-20.7762318	-18.0540600	-15.8687944	-13.0703888
	-24.1553593	-20.7343769	-15.9562664	-13.0767441	-9.6850843
END					

6.5 Modified HITRAN Line File

The augmented HITRAN[8] line file used by SHARC includes line parameters for 13 radiators: CO, OH, O_3, NO^+, NO, CH_4, four isotopes of H_2O and three isotopes of CO_2. The line file contains the spectral line information required to perform line-by-line emission calculations for each radiator. There are a total of more than 150,000 lines in the file. The lines in the file have been modified to speed up the LOS spectral radiance calculation. The first modification was to separate the total energy of the lower state, E", into vibrational, E_V, and rotational, E_R, components. SHARC requires the separate E_V and E_R to properly scale the line strength since the vibrational and rotational temperatures can differ. Computational time is saved by storing E" and E_R rather than re-calculating them in the spectral radiance module.

The standard HITRAN line strengths have also been modified. The temperature-dependent scaling factors evaluated at the reference temperature, T_s = 296 K, have been removed from the strengths. This modification speeds up the spectral radiance calculation by eliminating the calculations which depend on

T_s. Although the CPU savings realized by removing T_s is fairly small per line, a typical calculation uses thousands of lines and, therefore, the total savings can be significant. The line strength, SR, stored in the database is given by:

$$SR = S(T_s)\,Q_v(T_s)\,Q_r(T_s)\,Q_e(T_s)\,exp(C_2\frac{E''}{T_s})\,[1-exp(-(\quad (8)$$

where $S(T_s)$ is the standard HITRAN line strength, W_o is the transition wavenumber, I_a is the fractional isotopic abundance, and Q_v, Q_r, and Q_e are the vibrational, rotational, and electronic partition functions, respectively. C_2 is the second radiation constant (C_2 = 1.43879).

The following database parameters are used in the spectral radiance module of SHARC:

MOL - AFGL molecular species identification label
ISO - AFGL molecular species isotope identification label
W_o - transition frequency (cm^{-1})
SR - modified line strength (cm^{-1}/molecule/cm^{-2})
GAM - Lorentz halfwidth (cm^{-1})
E" - total energy of lower state (cm^{-1})
E_R - rotational energy of lower state (cm^{-1})
IUP - upper state vibrational label
ILOW - lower state vibrational label.

An example of the database is given in Table 9; we have included only the parameters currently used by SHARC. This part of the line file includes lines for three isotopes of H_2O (MOL=1), and the major isotope for O_3 (MOL=3), CH_4 (MOL=6), and OH (MOL=13).

Table 10 displays the eight (thirteen) currently supported molecular species (radiators) and their associated molecular identification labels. Note that number 29 is used for NO^+ here, but not in the AFGL system.

The line file used by SHARC is written in binary format. Using a binary representation of the file saves storage space and makes the reading time shorter than if the file were stored in an ASCII format. The file is provided on the SHARC computer tape or a Bernoulli disk in ASCII format along with a program which converts it to binary.

Table 9. Excerpt from the SHARC Line Parameter Database.

MOL	ISO	W_o	SR	GAM	E"	E_R	IUP	ILOW
3	1	325.023900	0.3141E-1	80.0718	959.2989	258.3679	5	2
3	1	325.043700	0.6928E-1	80.0709	903.2928	202.3618	5	2
6	1	325.089630	0.2298E-1	60.0440	2636.2571	1325.4965	2	2
1	1	325.141200	0.5015E-1	30.0687	3162.2590	1567.5090	2	2
3	1	325.164700	0.1081E-1	70.0751	841.3435	140.4125	5	2
3	1	325.183400	0.9109E-1	80.0712	865.7697	164.8387	5	2
3	1	325.218300	0.8106E-1	80.0706	880.9405	180.0095	5	2
6	1	325.273810	0.3529E-1	80.0510	2167.9641	857.2035	3	2
6	1	325.280200	0.2715E-1	80.0470	2473.1780	1162.4174	3	2
6	1	325.304880	0.7862E-1	90.0470	2473.3799	1162.6193	3	2
1	2	325.311000	0.1099E-1	50.0609	921.8950	921.8950	1	1
3	1	325.340400	0.4661E-1	80.0700	1377.0950	676.1639	5	2
6	1	325.377060	0.1288E-1	80.0360	2473.2439	1162.4833	3	2
6	1	325.449730	0.1109E-1	60.0280	3042.0859	1731.3253	2	2
3	1	325.524500	0.1016E-1	70.0746	841.2429	140.3119	5	2
1	2	325.554000	0.7320E-1	70.0502	2099.5620	2099.5620	1	1
3	1	325.568000	0.4849E-1	80.0701	1355.3521	654.4210	5	2
3	1	325.601800	0.4813E-1	80.0716	921.8952	220.9642	5	2
13	1	325.668700	0.1487E-1	50.0830	1367.6270	1241.3311	17	17
13	1	325.671300	0.2262E-1	30.0830	1367.6270	1241.3311	17	17
13	1	325.671300	0.2010E-1	30.0830	1367.6250	1241.3290	17	17
1	3	325.699000	0.2701E-1	60.0465	884.1140	884.1140	1	1
1	3	325.741000	0.8105E-1	60.0460	884.0780	884.0780	1	1
1	1	325.785400	0.1675E-1	20.0598	2398.3821	803.6321	2	2
3	1	325.792400	0.5056E-1	80.0702	1334.4430	633.5120	5	2

Table 10. SHARC Radiators and Identification Numbers.

CHEMICAL SPECIES	IDENTIFICATION NUMBER	ISOTOPE NUMBER
H_2O	1	1
H_2O	1	2
H_2O	1	3
H_2O	1	4
CO_2	2	1
CO_2	2	2
CO_2	2	3
O_3	3	1
CO	5	1
CH_4	6	1
NO	8	1
OH	13	1
NO^+	29	1

6.6 Model Atmosphere Files

A new SHARC-3 feature is SAG, the SHARC Atmosphere Generator.[22] It is discussed in Subsection 7.2 below. The previous SHARC atmospheric profiles, 1976 standard and subarctic summer, for day and night, are still furnished, although using SAG is recommended. These earlier profiles are based on a fairing of the AFGL standard profiles[25] and the HAIRM[26] atmospheric models. In addition, several atmospheric profiles produced by SAG are included for the multiple-profile test cases 4 and 5. These models include temperature and number densities for N_2, O_2, O, OH, CO_2, H_2O, NO, H, O_3, CH_4, and CO as a function of altitude. The profiles are layered into 65 homogeneous layers (66 layer boundaries) defined in 2 km increments from 50 to 150 km and in 10 km increments from 150 to 300 km.

The model atmosphere file is contained in an 80 column, format free ASCII file. The input file is checked for proper syntax and self-explanatory diagnostic messages are written to the SHARC journal file if unacceptable syntax is encountered.

The user can define a new atmosphere file by following a set of simple rules. A SHARC atmospheric file is structured as a series of input parameter identification lines followed by the actual input values (at least one) and an END line that denotes the end of the parameter input.

As an example, the daytime 1976 Standard Atmosphere Model input file provided with SHARC is shown in Appendix E. As the various input parameters are described, it should help the user to refer to this appendix.

The following input parameter identification lines must be contained in the user-defined atmospheric model file in the order listed:

- ATMOSPHERE NAME Line
- NUMBER OF LAYER BOUNDARIES Line
- DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE Line
- SPECIES Line
- ALTITUDES Line
- TEMPERATURES Line
- SPECIES DENSITIES Line.

Each input parameter identification line must start in Column 1. After the appropriate data corresponding to the identification line have been entered into the file in the next line, the line after next must contain the word END beginning in Column 1. The information required after each parameter identification line is detailed below.

The line following the ATMOSPHERE NAME line must contain the alphanumeric name of the atmospheric file being used. In the example, the name is DAY76.ATM. Up to 32 non-blank characters are allowed. If the name does not match the actual file name, a warning is entered into the SHARC.LOG file. After the END line (and following the NUMBER OF LAYER BOUNDARIES line), the number of layer boundary points should be entered. There must be at least 2 layer boundaries, and the current maximum is 66 boundaries, as in the example. To increase the maximum number of boundaries, the parameter NBYMAX defined in PARMS.H must be changed from 66 to the required value and SHARC must be re-compiled. Next, the DAY-NIGHT parameter and the EXOATMOSPHERIC TEMPERATURE should be defined exactly in the order stated and separated by at least one blank space. The DAY-NIGHT parameter is entered as either DAY (shown) or NIGHT. After the SPECIES line, a list of atmospheric species for which number densities are given is input. This list of species must include all molecular species desired in the model atmosphere. Eleven such appear in Appendix E, including O_2, N_2, O, and H, which are not SHARC radiators but are involved in the kinetics. The same rules apply to entering the atmospheric species as those given for the INTERPRETER (see Subsection 7.1.1). Also, each species listed in the atmosphere file must be listed as a species in the interpreter (originally, the kinetics) file. The ALTITUDES line precedes the next inputs considered, the altitudes of the layer boundaries. Any number of lines may be entered to define the layer altitudes. The altitudes must be entered in ascending order. The input units are km and are converted to cm for internal use. In the example, the altitudes come in rows of five, but this particular ordering is not necessary. The number of altitudes must match that specified earlier by the NUMBER OF LAYERS line, 66 here. Next, the kinetic temperatures and species number densities are entered in such a way as to correspond to the layer boundary altitudes. The number of entries for the temperatures and each species number densities must equal the value of the NUMBER OF LAYERS parameter. The temperatures are input in degrees Kelvin and the number densities are input in molecules/cm^3. After the line containing the END line for the TEMPERATURE data, a line with one of the valid atmospheric species names (followed by a blank and the word DENSITIES) indicates the beginning of the atmospheric number densities input for this species. Again, the data is followed by the word END beginning in Column 1. The procedure for the atmospheric species is continued until number densities have been defined for all atmospheric species listed in the SPECIES section of the file.

6.7 Data File Summary

To execute SHARC the user must first prepare several input files. Many of these files require no modification by the user unless the user desires to change and/or supplement the database provided with SHARC. The SHARC input and output files are summarized in Table 11. These files are:

- 15 Linking files (one for each molecular radiator),
- 15 States files (one for each molecular radiator),
- 12 Bands files (one for each molecular radiator, none required for auroral species),
- 12 Curtis-Godson bands files (one for each molecular radiator, none for auroral species),
- 1 Model atmosphere profile file (18 are provided),
- SHARC HITRAN file (binary version), and
- SHARC input file (SHARC.INP).

Table 11. Summary of the Files Used by SHARC.

LINKING	STATES	BANDS	Curtis-Godson	INPUT	OUTPUT
CO.LNK	CO.STA	CO.BND	CO.CGD	SHARC.INP	SHARC.LOG
NO.LNK	NO.STA	NO.BND	NO.CGD	SHARC.H92	SHARC.OUT*
O3.LNK	O3.STA	O3.BND	O3.CGD	DAY76.ATM%	SHARC.SPC*
OH.LNK	OH.STA	OH.BND	OH.CGD		SHARC.TRN*
CH4.LNK	CH4.STA	CH4.BND	CH4.CGD		POPNEW.DAT*
H2O1.LNK	H2O1.STA	H2O1.BND	H2O1.CGD		
H2O2.LNK	H2O2.STA	H2O2.BND	H2O2.CGD		
H2O3.LNK	H2O3.STA	H2O3.BND	H2O3.CGD		
H2O4.LNK	H2O4.STA	H2O4.BND	H2O4.CGD		
CO21.LNK	CO21.STA	CO21.BND	CO21.CGD		
CO22.LNK	CO22.STA	CO22.BND	CO22.CGD		
CO23.LNK	CO23.STA	CO23.BND	CO23.CGD		
ACO2.LNK	ACO2.STA				
ANO.LNK	ANO.STA				
ANOP.LNK	ANOP.STA				

% This is one of the 18 model atmosphere files supplied.
* User-supplied name.

The states, bands, and Curtis-Godson files are described in Subsections 6.2, 6.3, and 6.4 respectively. The linking files are generated by running the INTERPRETER and are described in Section 7. The states, bands, Curtis-Godson and model atmosphere files are provided with the code and require no modification. The binary SHARC HITRAN file is generated from an ASCII file provided on the SHARC computer tape. Forming this binary file and compiling/linking SHARC are described in Appendix A. Finally the SHARC input file, SHARC.INP, must be available to SHARC, or a new SHARC.INP will be created. The input module and the SHARC.INP files are described in Section 3.

7. AUXILIARY SHARC PROGRAMS

7.1 The INTERPRETER Program

The SHARC CHEMKIN module computes the steady-state and time-dependent number densities of vibrationally excited atmospheric species from a set of chemical kinetics/reaction mechanisms. The chemical kinetics mechanism describes molecular formation, all forms of vibrational energy transfer, and the absorption of solar and/or earthshine radiation. SHARC's access to the chemical kinetics mechanism and associated input (that is, energy transfer or reaction rate constants) is provided by a program called the INTERPRETER. The INTERPRETER reads the chemical kinetics data base and creates a binary "linking" file with this information. The SHARC INTERPRETER is based entirely on and includes subroutines directly from the Sandia Livermore INTERPRETER code which is provided with the CHEMKIN code.[6] The Sandia CHEMKIN package is described as "a general-purpose, problem-independent, transportable, FORTRAN chemical kinetics code."[6] The SHARC INTERPRETER is a modified Sandia interpreter from which information on elements in the periodic table and the thermodynamic data base (useful for combustion reactions, but extraneous to this application) has been removed.

Once the chemical kinetics mechanism has been formulated, the INTERPRETER provides the vehicle by which the information is transferred to the CHEMKIN module in SHARC. The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism in a manner that is just as would be written by a chemical kineticist; it then translates this information into the appropriate differential rate equations. Consider I irreversible kinetic (energy transfer or reactive) processes involving L species. Each process is expressed in the general form

$$\sum_{\ell=1}^{L} \nu(\ell,i)\, C_\ell \quad \overset{k_i}{\rightarrow} \quad \sum_{\ell=1}^{K} \nu'(\ell,i) \quad C_\ell \quad , \tag{9}$$

The stoichiometric coefficients of the ℓ^{th} species in the i^{th} process, $\nu(\ell,i)$, are integers. C_ℓ is the chemical symbol for the ℓ^{th} species; and k_i is the rate constant for the i^{th} process. The INTERPRETER reads this symbolic description of an arbitrary chemical kinetics mechanism and provides the data necessary to translate the mechanism into the appropriate differential equations for the production rates of the species. The production rate for the j^{th} species, $d[C_j]/dt$, is given by

$$\frac{d[C_j]}{dt} = \sum_{i=1}^{I} (\nu(j,i) - \nu'(j,i)) k_i \prod_{\ell=1}^{I} [C_\ell]^{\nu(\ell,i)} \qquad (10)$$

All the variables defined in Equations (9) and (10) are written into a binary "linking" file. Although this example is shown for irreversible processes, it should be noted that SHARC allows the use of reversible vibrational to translational processes. However, reversible vibrational to vibrational energy exchange processes must still be explicitly entered as irreversible reactions in the forward and reverse directions. The INTERPRETER only has to be run once for a given kinetics mechanism and data base. The "linking" file is then saved and used by SHARC for all subsequent calculations. Of course, if the kinetics mechanism or data base is changed, the INTERPRETER has to be rerun.

The INTERPRETER needs an ASCII input file named INTERP.INP, which contains the chemical kinetics mechanism for producing vibrationally excited states for the selected radiator. The structure for this input file is discussed below. After execution of the INTERPRETER, two output files are created: INTERP.OUT and INTERP.LNK. The file INTERP.OUT is an ASCII file and contains information from the input file. The user should check this file to ensure that the INTERPRETER was successfully executed. Any error messages created during program execution will be written to this file. The file INTERP.LNK is a binary file (that is, the "linking" file) which contains the chemical kinetics information required by SHARC. This file is only created if no errors were encountered during the INTERPRETER execution.

Twelve chemical kinetics mechanism input files are currently supplied with SHARC for CO, NO, O_3, OH, CH_4, four isotopes of H_2O, and three isotopes of CO_2. There are also auroral kinetic files for the primary isotope of CO_2, NO^+ and NO. The input file names are summarized in Table 12. In order to create a "linking" file for one of the radiators, say CO, one would proceed as follows:

(1) copy the file CO.KIN to INTERP.INP,

(2) execute the INTERPRETER,

(3) rename INTERP.OUT to CO.OUT, and

(4) rename INTERP.LNK to CO.LNK.

The file CO.LNK would then be used as the "linking" file for SHARC. This procedure must be carried out for each molecular radiator, each H_2O and CO_2 isotope being considered as a separate species. A UNIX script file, interp.run, performs these four steps for each molecular radiator automatically. This

file is provided with SHARC-3. The interp.run file assumes that the INTERPRETER executable file is called "interp".

Table 12. Files Used by the INTERPRETER.

INPUT	OUTPUT	LINKING
CO.KIN	CO.OUT	CO.LNK
NO.KIN	NO.OUT	NO.LNK
O3.KIN	O3.OUT	O3.LNK
OH.KIN	OH.OUT	OH.LNK
CH4.KIN	CH4.OUT	CH4.LNK
H2O1.KIN	H2O1.OUT	H2O1.LNK
H2O2.KIN	H2O2.OUT	H2O2.LNK
H2O3.KIN	H2O3.OUT	H2O3.LNK
H2O4.KIN	H2O4.OUT	H2O4.LNK
CO21.KIN	CO21.OUT	CO21.LNK
CO22.KIN	CO22.OUT	CO22.LNK
CO23.KIN	CO23.OUT	CO23.LNK
ACO2.KIN	ACO2.OUT	ACO2.LNK
ANO.KIN	ANO.OUT	ANO.LNK
ANOP.KIN	ANOP.OUT	ANOP.LNK

7.1.1 INTERPRETER Files

The INTERPRETER reads the symbolic description of a chemical kinetics mechanism from the INTERP.INP file and writes the information describing the mechanism to the INTERP.LNK file for subsequent use by the CHEMKIN module. The input required by the INTERPRETER is the species name used in the mechanism and the mechanism itself. An example of the CO chemical kinetics mechanism input file currently used by SHARC is given in Table 13.

The information contained in the input file is given in an 80-column format. All input to the INTERPRETER is format free. The INTERPRETER checks each input line for proper syntax and writes self-explanatory diagnostic messages to the output file if bad syntax is encountered. If any errors are encountered, the INTERPRETER does not create the linking file. Therefore, the input must be error free before SHARC can be executed.

The rules for creating the INTERPRETER input file have been described in detail elsewhere.[6] Subsection 7.1 reproduces this input procedure as previously described. Some changes to the information expected in the SHARC INTERPRETER input file are incorporated in these sections.

Table 13. SHARC INTERPRETER CO Kinetics Mechanism Input File.

```
CO SHARC CHEMICAL KINETICS MECHANISM
SPECIES
N2  O2  O  CO2  CO  H2O  NO  O3  H  OH
N2(0) N2(1)
CO(0) CO(1) CO(2) CH4
END
REACTIONS
M + CO(1)  =  M + CO(0)                  9.90E-09  0.0    168.1    0.0
    N2/1.0/  O2/1.0/
O + CO(1)  =  O + CO(0)                  2.82E-09  0.0    75.4     0.0
M + CO(2)  =  M + CO(1)                  1.98E-08  0.0    168.1    0.0
    N2/1.0/  O2/1.0/
O + CO(2)  =  O + CO(1)                  2.82E-09  0.0    75.4     0.0
O + CO(2)  =  O + CO(0)                  2.82E-09  0.0    75.4     0.0
CO(0) + N2(1)  -  CO(1) + N2(0)          6.98E-13  0.0    25.6     0.0
CO(1) + N2(0)  -  CO(0) + N2(1)          6.98E-13  0.0    25.6     268.5
CO(1)  -  CO(0) + HV                      30.96    0.0    0.0      0.0
CO(2)  -  CO(1) + HV                      60.45    0.0    0.0      0.0
CO(2)  -  CO(0) + HV                      1.03              0.0
0.0     0.0
CO(0) + HV  -  CO(1)                      0.0               0.0
0.0     0.0
CO(0) + HV  -  CO(2)                      0.0               0.0
0.0     0.0
CO(1) + HV  -  CO(2)                      0.0               0.0
0.0     0.0
END
```

7.1.2 Species Lines

Each chemical species must be identified on a Species Line (or lines). Any set of up to 10 characters can be used as a species name, which must begin with a letter. Species names of more than 10 characters may be used by simply changing a parameter value and some related format statements in the INTERPRETER. The primary purpose of the Species Lines is to identify the atmospheric species, the vibrational states included in the chemical kinetics mechanism for the selected radiating species, and finally the order in which arrays of species information are referenced in SHARC.

The first Species Line must contain the word SPECIES starting in Column 1. It is then followed by any number of lines that identify the species. Species symbols may appear anywhere on the line, and those on the same line must be separated by blank spaces. After all the species have been given, the following line must contain the word END starting in Column 1. The rules for Species Lines are summarized in Table 14.

Table 14. Summary of the Rules for Species Lines.

1. The first (last) species Line must contain the word SPECIES (END) starting in Column 1. All other columns on this line are ignored.
2. Species names are composed of up to 10-character symbols. The names cannot begin with the characters +, -, =, a parenthesis, or a number.
3. Each species must be declared only once.
4. Each species that subsequently appears in a reaction must be declared.
5. The species declarations may appear anywhere on the lines.
6. Any number of species declarations may appear on a line. More than one line may be used.
7. Species declarations that appear on the same line must be separated by at least one blank space.
8. A species declaration that begins on one line may not continue to the next line.
9. One species declaration may end in Column 80 of one line and the next declaration may begin in Column 1 of the next line.

7.1.3 Reaction Mechanism Description

The reaction mechanism involves a number of chemical reactions and/or energy transfer processes involving the species named on the Species Lines. The first Reaction Line must contain the word REACTIONS starting in Column 1. The following lines contain the reaction description together with the generalized Arrhenius/Schwartz-Slawsky-Herzfeld (SSH) rate coefficients. The reaction description is made up of Reaction Lines and perhaps Auxiliary Information Lines. The last line of the reaction description must contain the word END starting in Column 1.

7.1.3.1 Reaction Lines

Each Reaction Line is divided into two fields. The first field contains the symbolic description of the reaction while the second contains the Arrhenius/SSH rate coefficients. Both fields are format free, and blank spaces are ignored (except within a number or a species symbol). The reaction description, given

in the first field, must be composed of the species symbols, coefficients, delimiters, and special symbols as summarized below:

Species Symbols

Each species in a reaction is described with the unique sequence of characters exactly as they appear in the Species Lines.

Coefficients

Any species symbol may be preceded by an integer coefficient. The coefficient simply has the meaning that there are that many moles of the particular species present as either reactants or products; for example, 2OH is equivalent to OH + OH (non-integer coefficients are not allowed).

Delimiters

+	A plus sign is the delimiter between the reactant species and between the product species.
=	An equality sign is the delimiter between the reactants and products for a reversible reaction.
-	A minus sign is the delimiter between the reactants and products for an irreversible reaction.

Special Symbols

M	The symbol M stands for an arbitrary third body. Normally it would appear as both a reactant and a product. However, it has the identical meaning even if it appears only as a reactant or a product. An M anywhere in the reaction description indicates that a third body is participating in the reaction. In any reaction containing an M, species are specified to have third-body efficiencies, in which case the next line(s) must be Auxiliary Information lines (described below).
HV	The symbol HV indicates that photon radiation ($h\nu$) is present as either a reactant or a product. If an HV appears in a reaction description, the wavelength of the radiation may be specified on an Auxiliary Information Line (described later).
E	The symbol E is used to represent an electron. Electrons are treated just like any other species except that they are not composed of elements.
[	An open bracket means that any following characters through the beginning of the numbers for the Arrhenius coefficients are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

A special case for reaction descriptions occurs if two or more species names are identical except for the last character in one of the names being a +, -, or = (for example, NO, NO+). The INTERPRETER always seeks to find the longest possible species name between delimiters (+, -, =). Therefore, the species NO may not be followed directly by a + as a delimiter since this would be

confused with the species NO+. To prevent this confusion, the species NO must be separated from the delimiter + by at least one blank space (for example, the reaction NO+O+M = NO2+M must be written as NO +O+M = NO2+M). However, NO+ +E+M = NO +M may just as well be written as NO++M+E = NO +M as long as NO++ is not a species. There is no ambiguity in the convention, and the worst that can happen if the blank is not included before the delimiter is that an error message will be written from the INTERPRETER. The blank will have to be inserted by the user, but there is no possibility of having a reaction misinterpreted by the code and proceeding with an incorrect reaction.

The second field of the reaction line is used to define the Arrhenius/SSH rate coefficients A_i, β_i, C_i, and E_i. The rate constants are assumed to have the following functional form

$$k_i = A_i T^{\beta i} exp(-C_i / T^{1/3} - E_i / T) \quad . \tag{11}$$

The four numbers must appear in order: the first number being A_i, the second being β_i, the third being C_i, and the fourth being E_i. At least one blank space must separate the first number and the last symbol in the reaction or the comment. The four numbers must be separated by at least one blank space; be stated in either integer, floating point, or E format (for example, 123 or 123.0 or 12.3E1) and have units associated with them. The default units for A_i are cgs (cm, sec, K, and molecules), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the SSH parameters and activation energies are $K^{1/3}$ and K, respectively.

Table 15 is a summary of the Reaction Line rules, and examples of some reaction lines are shown in Table 13.

Table 15. Summary of the Rules for Reaction Lines.

1. The first (last) Reaction line must contain the word REACTIONS (END) starting in Column 1. All other columns on this line are ignored. (The END line would follow the last Auxiliary Information Line, if one was used for the last reaction).

2. The reaction description can begin anywhere on the Line. All blank spaces, except those within species symbols and within coefficients, are ignored.

3. If some species names end with either the characters +, -, or =, and there are other species names that are identical except that they do not end in a +, -, or =, then in the reaction description the latter species names must be separated from +, -, or = delimiters by at least one blank space.

4. Each reaction description must use only one line and may not continue onto the next line.

5. Four numbers for the Arrhenius/SSH coefficients must appear on each Reaction Line, must occupy the last non-blank entries on the line, must be separated from the reaction description by at least one blank space, must be in the order (A_i, β_i, C_i, and E_i), and must be separated by at least one blank space. No blanks are allowed within the numbers themselves.

6. Comments are any characters following an open bracket and up to within one blank space of the first Arrhenius coefficient. The comments are written on the output file along with the reaction description, but otherwise ignored within the code.

7.1.3.2 Auxiliary Information Lines

If a reaction contains an M as third body and/or it contains an HV to denote radiation, the line or lines following that reaction line may be Auxiliary Information Lines. These lines specify third-body efficiencies of certain species or specify radiation wavelength. Any species which acts as a third body must be declared as one of the species on the Species Lines.

The format of the line is a name (either a species name or the characters HV) followed by a number [either integer, floating point, or E format delimited by slashes(/)]. For enhanced third-body efficiencies, the name is the species name of the enhanced third body, and the number is its enhanced efficiency factor. For wavelength specification, the symbols HV are followed by the wavelength.

Any number of third-body efficiencies may be included, and each Auxiliary Information Line may contain one or more efficiency factors. If more than 6 species are to be specified as third bodies in any one reaction, some dimensioning needs to be changed in the INTERPRETER. Also, the radiation wavelength may appear on a separate line, or it may be on the same line as a third-body efficiencies

specification. Thus more than one Auxiliary Information Line may be used for any one reaction. Examples of auxiliary information are shown in Table 13. The above rules are summarized in Table 16.

Table 16. Summary of the Rules for Auxiliary Information Lines.

1. Auxiliary Information Lines may only follow Reaction Lines that contain an M or an HV.
2. A species may have only one third-body efficiency associated with it in any one reaction.
3. Only one radiation wavelength may be declared in a reaction.
4. The order in which the enhanced third-body declarations are given is the order in which arrays of third-body information are referenced in the subroutine package. The order in which the radiation wavelength appears with respect to enhanced third-body information is unimportant.
5. Third-body (or wavelength) information may appear anywhere on the line.
6. Any number of third-body efficiencies may appear on a line. More than one line may be used.
7. Third-body declarations or radiation wavelength specifications that appear on the same line must be separated by at least one blank space.
8. A third-body (or wavelength) declaration that begins on one line may not continue on to the next line.
9. One declaration (third-body efficiency or wavelength) may end in column 80 of one line, and the next declaration may begin in Column 1 of the next line.
10. Any blank spaces between the species symbol (or HV) and the first slash are ignored, and any blanks between the slashes and the efficiency factor (or wavelength) are also ignored. However, no blank spaces are allowed within the factor (or wavelength).

7.1.3.3 Reaction Mechanism Format Summary

As indicated the reaction mechanism may involve any number of chemical reactions and/or energy transfer processes involving the species named on the Species Lines. If more than six species appear in a given reaction, some dimension statements in the INTERPRETER must be changed. In the INTERPRETER for SHARC-1, the energy transfer/reactive processes were written explicitly in the forward and/or reverse directions. In later versions, however, vibrational-to-translational energy transfer

processes may be written in the forward direction (with reactants and products separated by the delimiter "=" rather than "-"). SHARC then computes the reverse rate constant using detailed balance. Vibrational-to-vibrational energy transfer processes must still be written explicitly in the forward and reverse direction. Processes may be three-body reactions with an arbitrary third body including the effects of enhanced third-body efficiencies, or may involve radiative relaxation and/or excitation (for example, earthshine and/or sunshine).

7.2 Required Correspondences Between Data Files

The data files supplied with SHARC-3 are mutually consistent, supplying all the information needed for each radiator with the chosen kinetics scheme. In modifying these files to support an extended or new kinetics or set of states and transitions, the user must insure that changes are made in all the files which require change. Requirements for the individual files have been discussed above; this section points out how to keep data files consistent after modifications.

The kinetics file both establishes the kinetic scheme and constrains the effect that the states and bands files can have. A state or transition which is not called out here will not contribute to the calculation, and if added to the states or bands file it will generally result in an error, warning or caution printed to the SHARC.LOG file. When a transition is added to the kinetics file, both the forward and the reverse processes must be added. Vibration-translation processes are excepted. The user should remember that, unlike the case for the states and bands files, a change to the kinetics file alone does not affect SHARC calculations; after the change, the INTERPRETER must be used to generate the binary linking file. The derived linking file, not the source kinetics file, is what SHARC reads and uses.

The states and transitions in the states file should ideally match those in the kinetics file one to one. The bands file must then also acquire new bands corresponding to the new transitions, with each new band having all lines pertaining to that transition. Finally, the Curtis-Godson file should receive the same new bands as the bands file.

It is highly recommended that any changes follow this rule of one to one correspondence, with new states and transitions/bands appearing also in the kinetics file, even with zero rate constants.

SHARC will nonetheless run successfully for some departures from this rule. If a states-file line for a new energy is added, SHARC will run, with no messages commenting on the addition, and the results will be unchanged. If also, a states-file transition involving that new state is added, the run will terminate with an error message noting that the state is not in the species list of the linking file (derived from the kinetics file).

If a new transition is placed in the kinetics file but omitted from the states file, while the new state's energy is included in the states file, SHARC will run to completion. However, the new transition will have no impact on the output. The states-file transition line is needed before SHARC will include that transition.

Once a new state and one or more of its transitions have been placed correctly in the linking and states files, the bands file must be updated; a missing transition here will stop SHARC with an error message. The lines occurring in each new transition must be sorted into the appropriate strength bins as discussed previously. As was the case for an extra energy line in the states file, an extra band in the bands file will result in a successful run with no change to the output. In this case, however, a caution will be written noting that any new energy level involved in the band does not appear in the kinetics file. If, in addition, the new states are added to the states and linking file, an error will result.

Finally, solar absorptance by the lower atmosphere is defined by the Curtis-Godson files. Any change in the bands file, in either the transitions considered, or in the specific bins within a transition, must be reflected in corresponding changes in the Curtis-Godson files, or SHARC will stop with an error, such as:

```
ERROR IN LOWIN...
    MISMATCH IN BIN NUMBER FOR THE   CO(1)  - CO(0)          BAND
```

This is a message from SHARC. The name of the Curtis-Godson file is created by appending the string ".CGD" to the molecular formula. A missing Curtis-Godson file will be evidenced by a FORTRAN runtime error, such as:

```
Fortran runtime error on external file "kindir/CO.CGD" (2):
   No such file or directory
```

resulting from an attempt to open the nonexistent file. The above is a message from the FORTRAN compiler; SHARC does not check for the existence of the file before trying to open it. The exact message would depend on the compiler used. Note, SHARC will attempt to use this file only if the solar zenith is between 90° and 108°.

In brief, partial modifications to the SHARC data files may result in an apparently successful run, perhaps with warning or caution messages, which does not express the kinetic scheme the user intended. Most such modifications result in an error message and an incomplete calculation. The best policy is to make only complete changes. To do so, the user should check that a new energy is added to both the

kinetics and states file, a new transition to all four files, and that the linking file has in fact been compiled from the current kinetics file.

7.3 The SHARC Atmosphere Generator (SAG)

7.3.1 Purpose and Description

SAG generates a SHARC-compatible input file of atmospheric species and kinetic temperature profiles.[22] It is currently implemented as a stand-alone, interactive FORTRAN program. The profiles are customized for the geophysical and geographic information input by the user. From information on the date, time, location, and geomagnetic and solar activity, SAG accounts for systematic variabilities in CO_2, O_3, OH, NO, H_2O, and O atom densities, including terminator effects. For other species, SAG utilizes diurnally-averaged profiles from recent databases. To facilitate use without detailed inputs, defaults are provided so that simple designations, such as day/night, season, latitude region (low, mid, or high), etc., can be specified as desired.

SAG draws primarily on two existing atmosphere models. The empirical model MSISE-90[27] is used for the temperature and major species profiles. It provides profiles for species including N_2, O_2, O, and H as a function of altitude, latitude, longitude, universal time (UT), local solar time (LST), daily Ap, F10.7, and F10.7A (30 day average).

The second atmosphere model used extensively in SAG is a new NRL database[28] for altitudes up to 120 km. It contains mean monthly species concentrations at 1 to 5 km increments and 10^o latitude increments. SAG interpolates between these values and converts to number densities using the MSISE-90 total densities. This database is used for the SHARC species CH_4 and CO and for lower portions of the O_3 and O profiles, as well as for the additional species N_2O, NO_2 and HNO_3. The latter three species, among others, are included in the SHARC And MODTRAN MERGED (SAMM) code.[29] SAG has been designed to be compatible with the species and altitude ranges of SHARC, SAMM and MODTRAN.

The remaining profiles in SAG, including those for CO_2, NO, H_2O, OH, SO_2 and NH_3, are derived from a combination of standard concentrations[25] used in LOWTRAN and MODTRAN, from photochemical or empirical models based on MSISE-90 inputs or outputs, or from some combination of these.

The transition between the day and night profiles is handled using a simple empirical model that approximates the terminator behavior in the time-dependent calculations of Rodrigo et al.,[30] which were performed for mid-latitude equinox conditions above 60 km. The transition is made by linearly

interpolating over a 5° range of solar zenith angle (SZA) computed for LST-0.075 hr; the 0.075 hr (4.5 min) difference accounts for the approximate photochemical lag time. The midpoint of the interpolation region is taken to vary linearly with altitude at the rate of 0.12° per km. Based on a comparison with Rodrigo et al.'s calculations, this representation of the terminator location and width should be accurate to within around 1° in SZA in the 70-100 km altitude region.

7.3.2 Use and Operation

7.3.2.1 Menus

A main menu and two sub-menus are provided; they are largely self-explanatory. In the main menu, the user responds by typing an integer. The main menu reappears or a sub-menu appears following the user's response.

When SAG is run, the variables saved from the previous run (in file "drivstor.dat") are loaded into the menus. New parameter values are entered using the two sub-menus. The Parameter Menu is used to enter numerical values, such as would pertain to a specific experimental measurement. Upon return to the main menu, a complete listing of the current parameters is given. The Default Menu is used for entering generic values. For example, the generic value of 35° latitude is entered when the latitude default designation "m" (mid-latitude) is entered. An "m" will then appear as the default value in the menu listing. If no default value is currently in use, none will appear in the listing. To display the numerical value corresponding to a default selection, enter the Parameter Menu.

One can re-enter any parameter or menu any number of times. By using both sub-menus, any combination of default parameters and directly entered parameters can be chosen.

Certain parameters in the Parameter Menu are mutually dependent. For example, UT and LST are mutually dependent for a given longitude. After specifying the longitude, either UT or LST should be entered; the program will then automatically update the other parameter. The solar zenith angle (SZA) is also a dependent variable, being a function of the longitude, latitude, Julian day, and either LST or UT. The program automatically calculates and updates SZA when any of those parameters are changed. SZA can also be directly entered, in which case the longitude is recomputed from the other variables.

7.3.2.2 Altitude List and SAMM Species Option

The altitudes and the choice of SHARC or SAMM species are specified in the "drivht" files called by the Default Menu. User-defined altitudes can be input via the file "drivht.dat." Line 1 contains an integer argument, 0 for outputting SHARC species only, 1 for all SAMM (SHARC plus MODTRAN) species. The number of altitudes appears on line 2. Up to 200 altitudes from 0 to 300 km are allowed; however, the minimum altitude the for SHARC-3 option is 50 km. The altitude list starts on line 3; FORTRAN general input format is used, so that either integer or floating point numbers may be entered.

7.3.2.3 List of Files

The files comprising SAG as supplied with SHARC-3 are as follows:

Main program file: Sag.f (or other name)

5 input files:
drivstor.dat (updated by SAG)
drivht.sha
drivht.sam
drivht.mod
drivht.dat (user-specified)

10 NRL data files in subdirectory NRLDAT:

CH4.NRL	CO.NRL	H2O.NRL
HNO3.NRL	N2O.NRL	NO2.NRL
O3D.NRL	O3R.NRL	OAT.NRL
TEMP.NRL		

Total files = 16.

In addition, the "drivstor" files used to generate the Test 4 and Test 5 atmospheres are included along with these atmospheres. Copying one of these to "drivstor.dat" permits duplication of the corresponding atmosphere. This, in turn, can serve as a starting point for modified atmospheres. See Appendix A for a complete list of supplied files.

7.4 The DEGRAD Program

The DEGRAD program is used to degrade the spectral resolution of SHARC's spectral radiance and transmittance data. DEGRAD is an internal SSI code delivered as a courtesy. DEGRAD accepts as input

the SHARC spectral radiance and spectral transmittance files, and enables the user to pass any of a variety of filter functions over the data. The program interactively prompts the user for all required inputs using a menu driven system. Default inputs are stored in a DEGRAD.INP file; if no such file exists, one is created when the program is executed.

8. REFERENCES

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APPENDIX A

IMPLEMENTATION INSTRUCTIONS

SHARC, version 3.0 of the Strategic High-Altitude Radiance Code, is furnished with the FORTRAN source code, input data sets, and five test cases. The code calculates the spectral radiance from 250 to 10000 cm^{-1} for arbitrary geometries from 50 to 300 km. SHARC includes radiance from CO_2, H_2O, NO^+, NO, O_3, OH, CO, and CH_4.

The tape contains 164 files. There are 11 major fortran files for SHARC, together with 10 fortran header files which are shared among the 11 major files. The interpreter has one fortran file as does the atmospheric generator. Two additional fortran files contain the ASCII to binary and binary to ASCII lines file conversion programs.

The others consist of 18 model atmosphere files, 54 data files for the seven current ambient molecular radiators, and the three auroral radiators, 15 interpreter output files, 1 ASCII line position and strength file, 26 files used by the atmospheric generator, and 5 input and output files for each of the five SHARC test cases.

The files are:

SHARC-3 SOURCE CODE

	Major routines		
1	sharc3.f	Main program	FORTRAN
2	ambien.f	Ambient environment	FORTRAN
3	aurora.f	Auroral environment	FORTRAN
4	chmkin.f	CHEMKIN subroutines	FORTRAN
5	geolos.f	LOS Geometry subroutines	FORTRAN
6	geoseg.f	Segment Geometry subroutines	FORTRAN
7	inactv.f	Interactive subroutines	FORTRAN
8	input.f	Input subroutines	FORTRAN
9	inutil.f	Input Utilities subroutines	FORTRAN
10	output.f	Output subroutines	FORTRAN
11	spctra.f	Spectral Radiance subroutines	FORTRAN
		Shared Header files	
12	AMBIEN.H	Commons for Ambient Calculations	FORTRAN
13	DIRPKA.H	Commons for File names and directories	FORTRAN
		Population, kinetics and atmospheric profiles	
14	FILES.H	Common for file unit assignments	FORTRAN
15	ISOTP.H	Common for isotopic arrays	FORTRAN

16	KNETIC.H	Commons for chemical kinetics	FORTRAN
17	LOSGEO.H	Commons for LOS geometry variables	FORTRAN
18	PARMS.H	Shared parameters and array dimensions	FORTRAN
19	RADMAR.H	Commons for excited states indexing	FORTRAN
20	RECORD.H	Common for character string defaults	FORTRAN
21	REGGEO.H	Commons for region geometry and LOS/region intersections	FORTRAN

SUPPORTING SOURCE CODES

1	interp.f	CHEMKIN Interpreter program	FORTRAN
2	binary.f	Program to convert line data base from ASCII to binary	FORTRAN
3	ascii.f	Program to convert line data base from binary to ASCII	FORTRAN
4	sag.f	Atmosphere generation routines	FORTRAN
5	degrad.f	Slit function routines	FORTRAN

MODEL ATMOSPHERES

1	DAY76.ATM	1976 Standard Day	DATA
2	NIG76.ATM	1976 Standard Night	DATA
3	DSUBAR.ATM	Subarctic Summer Day	DATA
4	NSUBAR.ATM	Subarctic Summer Night	DATA
5	T4Z102.ATM	High Latitude Terminator	DATA
6	T4Z101.ATM	High Latitude Terminator	DATA
7	T4Z99.ATM	High Latitude Terminator	DATA
8	T4Z97.ATM	High Latitude Terminator	DATA
9	T4Z95.ATM	High Latitude Terminator	DATA
10	T4Z93.ATM	High Latitude Terminator	DATA
11	T4Z91.ATM	High Latitude Terminator	DATA
12	T5Z108.ATM	High Latitude Terminator	DATA
13	T5Z105.ATM	High Latitude Terminator	DATA
14	T5Z102.ATM	High Latitude Terminator	DATA
15	T5Z99.ATM	High Latitude Terminator	DATA
16	T5Z97.ATM	High Latitude Terminator	DATA
17	T5Z94.ATM	High Latitude Terminator	DATA
18	T5Z91.ATM	High Latitude Terminator	DATA

SPECIES DATA FILES

1	CH4.BND	CH_4 Band Information file	DATA
2	CH4.KIN	CH_4 Kinetics file	DATA
3	CH4.STA	CH_4 Transitions and state file	DATA
4	CH4.CGD	CH_4 Curtis-Godson file	DATA
5	CO21.BND	CO_2 Band Information file for 1st isotope	DATA
6	CO21.KIN	CO_2 Kinetics file for 1st isotope	DATA
7	CO21.STA	CO_2 Transitions and state file for 1st isotope	DATA
8	CO21.CGD	CO_2 Curtis-Godson file for 1st isotope	DATA
9	CO22.BND	CO_2 Band Information file for 2nd isotope	DATA
10	CO22.KIN	CO_2 Kinetics file for 2nd isotope	DATA
11	CO22.STA	CO_2 Transitions and state file 2nd isotope	DATA
12	CO22.CGD	CO_2 Curtis-Godson file for 2nd isotope	DATA
13	CO23.BND	CO_2 Band Information file for 3rd isotope	DATA
14	CO23.KIN	CO_2 Kinetics file for 3rd isotope	DATA
15	CO23.STA	CO_2 Transitions and state file for 3rd isotope	DATA
16	CO23.CGD	CO_2 Curtis-Godson file for 3rd isotope	DATA
17	CO.BND	CO Band Information file	DATA
18	CO.KIN	CO Kinetics file	DATA
19	CO.STA	CO Transitions and state file	DATA
20	CO.CGD	CO Curtis-Godson file	DATA
21	H2O1.BND	H_2O Band Information file for 1st isotope	DATA
22	H2O1.KIN	H_2O Kinetics file for 1st isotope	DATA
23	H2O1.STA	H_2O Transitions and state file for 1st isotope	DATA
24	H2O1.CGD	H_2O Curtis-Godson file for 1st Isotope	DATA
25	H2O2.BND	H_2O Band Information file for 2nd Isotope	DATA
26	H2O2.KIN	H_2O Kinetics file for 2nd Isotope	DATA
27	H2O2.STA	H_2O Transitions and state file for 2nd Isotope	DATA
28	H2O2.CGD	H_2O Curtis-Godson file for 2nd Isotope	DATA
29	H2O3.BND	H_2O Band Information file for 3rd Isotope	DATA
30	H2O3.KIN	H_2O Kinetics file for 3rd Isotope	DATA
31	H2O3.STA	H_2O Transitions and state file for 3rd Isotope	DATA
32	H2O3.CGD	H_2O Curtis-Godson file for 3rd Isotope	DATA
33	H2O4.BND	H_2O Band Information file for 4th Isotope	DATA

34	H2O4.KIN	H_2O Kinetics file for 4th Isotope	DATA
35	H2O4.STA	H_2O Transitions and state file for 4th Isotope	DATA
36	H2O4.CGD	H_2O Curtis-Godson file for 4th Isotope	DATA
37	NO.BND	NO Band Information file	DATA
38	NO.KIN	NO Kinetics file	DATA
39	NO.STA	NO Transitions and state file	DATA
40	NO.CGD	NO Curtis-Godson file	DATA
41	O3.BND	O_3 Band Information file	DATA
42	O3.KIN	O_3 Kinetics file	DATA
43	O3.STA	O_3 Transitions and state file	DATA
44	O3.CGD	O_3 Curtis-Godson file	DATA
45	OH.BND	OH Band Information file	DATA
46	OH.KIN	OH Kinetics file	DATA
47	OH.STA	OH Transitions and state file	DATA
48	OH.CGD	OH Curtis-Godson file	DATA
49	ACO2.KIN	CO_2 Auroral Kinetics file for 1st isotope	DATA
50	ACO2.STA	CO_2 Auroral transitions and state file for 1st isotope	DATA
51	ANO.KIN	NO Auroral Kinetics file	DATA
52	ANO.STA	NO Auroral Transitions and state file	DATA
53	ANOP.KIN	NO+ Auroral Kinetics file	DATA
54	ANOP.STA	NO+ Auroral Transitions and state file	DATA

INTERPRETER OUTPUT

1	CH_4.OUT	CH_4 output	DATA
2	CO21.OUT	CO_2 output for 1st isotope	DATA
3	CO22.OUT	CO_2 output for 2nd isotope	DATA
4	CO23.OUT	CO_2 output for 3rd isotope	DATA
5	CO.OUT	CO output	DATA
6	H_2O1.OUT	H_2O output for 1st isotope	DATA
7	H_2O2.OUT	H_2O output for 2nd isotope	DATA
8	H_2O3.OUT	H_2O output for 3rd isotope	DATA
9	H_2O4.OUT	H_2O output for 4th isotope	DATA
10	NO.OUT	NO output	DATA

11	O3.OUT	O_3 output	DATA
12	OH.OUT	OH output	DATA
13	ACO2.OUT	CO_2 Auroral output	DATA
14	ANO.OUT	NO Auroral output	DATA
15	ANOP.OUT	NO+ Auroral output	DATA

LINE DATA FILE

1	SHARC.ASC	ASCII line parameter file	DATA

ATMOSPHERE GENERATOR DATA FILES

1	drivht.sha	Input SHARC boundary altitudes	DATA
2	drivht.sam	Input SAMM boundary altitudes	DATA
3	drivht.mod	Input MODTRAN boundary altitudes	DATA
4	drivht.mos	Input MOSART boundary altitudes	DATA
5	drivstor	Current input parameter values	DATA
6	drT4Z102.dat	Test Case 4 input parameters	DATA
7	drT4Z101.dat	Test Case 4 input parameters	DATA
8	drT4Z99.dat	Test Case 4 input parameters	DATA
9	drT4Z97.dat	Test Case 4 input parameters	DATA
10	drT4Z95.dat	Test Case 4 input parameters	DATA
11	drT4Z93.dat	Test Case 4 input parameters	DATA
12	drT4Z91.dat	Test Case 4 input parameters	DATA
13	drT5Z108.dat	Test Case 5 input parameters	DATA
14	drT5Z105.dat	Test Case 5 input parameters	DATA
15	drT5Z102.dat	Test Case 5 input parameters	DATA
16	drT5Z99.dat	Test Case 5 input parameters	DATA
17	drT5Z97.dat	Test Case 5 input parameters	DATA
18	drT5Z94.dat	Test Case 5 input parameters	DATA
19	drT5Z91.dat	Test Case 5 input parameters	DATA
20	CH4.NRL	NRL database file for CH_4	DATA
21	CO.NRL	NRL database file for CO	DATA
22	H2O.NRL	NRL database file for H_2O	DATA
23	O3D.NRL	NRL database file for O_3	DATA
24	O3R.NRL	NRL database file for O_3	DATA
25	OAT.NRL	NRL database file for O atoms	DATA
26	TEMP.NRL	NRL database file for temperature	DATA

FIRST TEST CASE

1	SHARC1.IN	Input file	DATA
2	SHARC1.LOG	Journal file (empty)	DATA
3	TEST1.OUT	General output file	DATA
4	TEST1.SPC	Spectral file	DATA
5	TEST1.TRN	Transmission file	DATA

SECOND TEST CASE

1	SHARC2.INP	Input file	DATA
2	SHARC2.LOG	Journal file	DATA
3	TEST2.OUT	General output file	DATA
4	TEST2.SPC	Spectral file	DATA
5	TEST2.TRN	Transmission file	DATA

THIRD TEST CASE

1	SHARC3.INP	Input file	DATA
2	SHARC3.LOG	Journal file	DATA
3	TEST3.OUT	General output file	DATA
4	TEST3.SPC	Spectral file	DATA
5	TEST3.TRN	Transmission file	DATA

FOURTH TEST CASE

1	SHARC4.INP	Input file	DATA
2	SHARC4.LOG	Journal file (empty)	DATA
3	TEST4.OUT	General output file	DATA
4	TEST4.SPC	Spectral file	DATA
5	TEST4.TRN	Transmission file	DATA

FIFTH TEST CASE

1	SHARC5.INP	Input file	DATA
2	SHARC5.LOG	Journal file (empty)	DATA
3	TEST5.OUT	General output file	DATA
4	TEST5.SPC	Spectral file	DATA
5	TEST5.TRN	Transmission file	DATA

The FORTRAN source code for SHARC is found in the first 21 files. The files should be compiled and linked to make the executable version. All open statements for external files are in the main module, sharc3, the interactive menu module, inactv, and its utilities module, inutil. The SHARC subroutines are listed in Appendix C, and execution of SHARC is described in Sections 3 and 4.

The INTERPRETER should be compiled as a stand-alone program. INTERPRETER subroutines are described in Appendix B, and use of the program is discussed in Section 7.

The routine called binary converts the ASCII line parameter file shipped on the tape to a binary form for SHARC. Binary should be compiled as a stand-alone program. When binary is executed it reads a file called SHARC.ASC and outputs a binary version of the file. The new file is called SHARC.H92. The conversion of SHARC.ASC to SHARC.H92 needs to be performed only once. A program ascii.f can be compiled and executed to create an ASCII copy of SHARC.H92 if needed for installing on another machine.

APPENDIX B

INTERPRETER SUBROUTINES

The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism and translates it into the appropriate differential equations. The output from the INTERPRETER used by SHARC is a binary "linking" file which contains all the information describing the kinetic mechanism for a given molecular radiator.

A list of the subroutines comprising the INTERPRETER with a brief description follows.

MAIN — MAIN opens the input and output files used by the INTERPRETER, and defines the following parameters used to set the maximum size of storage arrays:

KMX	(=100)	The maximum number of species allowed during the execution of the INTERPRETER.
LENSYM	(=15)	The maximum length of a species symbol.
MAXSP	(=8)	The maximum number of species allowed in any given reaction.
MAXTB	(=6)	The maximum number of third bodies allowed in any given reaction.
NRCOF	(=4)	The number of parameters describing the reaction rate constant.
MXLEN	(=80)	The maximum length of an input string.
MXLENR	(=60)	The maximum length of a reaction input string.

CKINTP is the driver routine which reads the species and reaction mechanism input, checks for proper syntax, and writes the "linking" file.

CKTBD checks to make sure that different third-body efficiency factors have not been input for any species.

CKINTC converts a character input string into internal code.

CKNUM converts a character string into a specified number of real numbers. The character string may contain integer, floating point, or exponential numbers separated by at least one blank.

CKSCAN scans a character string (in internal code) and converts all digits into integer numbers and all species into species indices.

CKPARS checks the input string for format errors (that is, it enforces the rules given in Subsection 3.1)

CKERR writes the error messages into the output file.

APPENDIX C

SHARC SUBROUTINES

A list of the key dimensional variables and subroutines comprising the various SHARC fortran files listed in Appendix A is given below.

sharc3.f Main program and control of computations

The SHARC MAIN routine passes the name of the input file, normally SHARC.INP, to the top level subroutine, SHARC3. The SHARC3 routine obtains the input either in interactive or batch mode, calls the ambient and auroral chemistry modules, and then the LOS specification and radiation transport modules. It handles the selection of input/output files. The PARMS.H header file is included in SHARC3 and defines the following parameters to specify the size of various arrays.

VARIABLE	VALUE	DEFINITION
NAMLMX	32	Maximum number of characters for input/output file names.
NBINMX	10001	Maximum number of radiance bins (SPCRAD).
NBMAX	46	Maximum number of bands.
NBYMAX	66	Maximum number of layer boundaries.
NCHMAX	80	Maximum length of reaction input string.
NDMAX	400	Maximum number of lines in the defaults file.
NEDGE	4	Number of region edges.
NEDGMX	4	Maximum number of region edges.
NENVMX	2	Maximum number of environments for each region (ambient and auroral)
NFILES	3	Number of types of kinetics files (linking, states, bands).
NFIX	36	First NFIX data lines in the input file, defining information expected in the same sequence in every input file.
NIMAX	750	Maximum number of reactions.
NISOMX	8	Maximum number of isotopes for each species.
NKMAX	95	Maximum number of species allowed.
NLNMAX	15	Maximum length of a species symbol.
NMMAX	30	Maximum number of atmospheric species.
NMOL	29	Maximum number of molecules.
NMOLMX	8	Maximum number of distinct radiating molecules.
NRDMX	16	Maximum number of molecular emitters.
NREGMX	5	Maximum number of regions.
NSECMX	4	Maximum number of LOS intersections per region.

VARIABLE	VALUE	DEFINITION
NSMAX	20	Maximum number of bins for band distributions.
NSPMAX	8	Maximum number of species allowed in any given reaction.
NSTRMX	72	Maximum number of characters in a character string in the defaults file.
NTBMAX	6	Maximum number of third bodies allowed in any given reaction.
NTMPMX	5	Maximum number of temperatures for band distributions.
NVARMX	20	Maximum number of variables for generic interactive read.
NVMAX	35	Maximum number of vibrational states for each molecular emitter.

NWMAX	200	Number of frequency bins for the Voigt line shape function (NEMESIS).
NWMAX	200	Maximum number of frequency bins for the Voigt line shape function (NEMESIS).
NWUSED	10	Maximum number of items presently expected to be read from a single line of the input file.
NWRTMX	20	Maximum number of types of output.

Several additional parameters are related to the above parameters and are automatically adjusted when the above parameters are changed. For example, the maximum number of altitude layers and the maximum number of LOS segments are related to the maximum number of layer boundaries and the maximum number of regions.

inactv.f — Major routines of the interactive module

ADDRAD is the input routine which is used to add radiative species to the ambient and auroral population calculations.

ADDREG is the routine for reviewing, editing and adding regional information.

ALLOLD determines whether or not all population files are old.

CHKLYR checks that sets of boundary altitudes of multiple profiles within a region are the same.

CHKPOP compares population file content information for consistency with region data and other profiles specified in SHARC.INP.

CHKREG checks all regional information, such as filenames and input variable prior to an calculation.

GENTAB generates the proper character string for appending to a standard population file name.

INATM is the interactive input routine for reviewing/changing the user's choice of model atmosphere.

INAUR is the interactive input routine for reviewing/changing the user's choice of auroral conditions.

INBOND is the interactive input routine for inputing the parameters which define a local region.

INMOL is the interactive input routine for reviewing/changing the radiators included in the population calculations.

INNAME is the interactive input routine for reviewing/changing the names for the standard input and output files.

INNEM	is the interactive input routine for reviewing/changing the input parameters for the Monte Carlo radiation trapping module.
INOUT	allows the user to review and/or modify the amount of output written to the general output file.
INPOP	is the interactive input routine for reviewing/changing the population file names and status.
INREGN	is the main interactive input routine for reviewing/changing regional information.
INSOL	is used to change/review the solar zenith angle.
INSPEC	is the interactive input routine used to change and/or modify the spectral range, resolution and species included in spectral radiance calculation.
INSTDS	supplies the menus for input of name patterns and directories for kinetics, atmospheric, population and lines files.
INTITL	is the interactive input routine for reviewing/changing the title of the calculation.
INTYPE	is the interactive input routine used to change the environment type. SHARC currently has two environments: ambient and auroral.
POLL	contains the main interactive menu for running SHARC.
PROBDF	is the main driver for the interactive menu or batch execution of SHARC. This routine determines all of the input parameters for a sharc calculation.
RMRAD	eliminates a radiator from the list of species desired for population calculation.
RMREG	is used to remove an unwanted region.
SPCCHK	checks to ensure that populations exist for all species selected for spectral calculation.

input.f — Non-interactive input routines

BLOCK DATA	is located in the INPUT Module and sets numerous parameters concerning molecular data.
ATMDEN	loads atmospheric profile into the appropriate local arrays.
ATMIN	identifies the atmospheric species in the general species list, and reads atmospheric profile (containing the species number densities and kinetic temperature).
ATMLYR	computes the atmospheric properties for each layer.

ATMSYM	sets up the character arrays identifying the atmospheric species and an indexing array which relates the atmospheric species to the species read by CKLINK.
BANDIN	reads the molecular bands file (Subsection 3.3), which describes the line strength distribution function parameters for each vibrational transition.
BOTCHK	checks that the lowest altitude in an atmospheric profile matches that defined in block data. This assures consistency within the layer to layer pumping routine.
CKLINK	reads the "linking" file created by INTERP, and defines the arrays containing information on species names, chemical kinetics mechanism (that is, the stoichiometric coefficients and the rate constants).
DATE	calls a system-dependent routine to determine the date and time of the SHARC run. The actual call is commented out of the subroutine.
LOWIN	reads the Curtis-Godson files for lower-atmosphere solar radiation propagation.
POPIN	reads in population file data for CHKPOP.
RADIN	reads the molecular states file (Subsection 3.2), which contains the molecular radiator, the vibrational states included in the mechanism and the transitions to be considered by NEMESIS and SPCRAD.
REGCHK	checks region altitude boundaries for consistency with profile boundaries.
RETREV	reads the saved population file data.
XNUM	translates an alphanumeric character string containing N integer, real, or exponential numbers into their respective real values.

inutil.f — Input utilities routines

ACTIVE	reads the first data line in the default file to determine if the calculation is interactive or batch.
CATSTR	is a utility for concatenating two strings.
COMOUT	prints standard comments into the defaults file.
DFLTSG	reads the regional information found in the defaults file.
CPYSTR	is a utility for copying character strings.
DCHECK	checks for the existence of a directory.
DUMPDE	writes the current values of the input variables into the defaults file.

FCHECK	opens files and checks their status against the expected status. For example, does a new file already exist.
ITOASC	converts an integer to its ASCII representation.
KEEPI	stores a copy of an integer vector.
KEEPR	stores a copy of a real vector.
LENSTR	determines the non-blank length of a character string.
LOADDE	opens and loads the input data found in SHARC.INP into the array DFLTS. If SHARC.INP is not found, NODFTS is called to load a set of default parameters.
LOCASE	converts a character string to lower case.
MCHECK	checks the range of the variable to verify that the variable value is between the given bounds.
MRGSTR	merges a character string with another string.
NODFTS	loads the default values for a calculation into SHARC.INP when an SHARC.INP is not found.
PARSEC	separates text and numerical input parameters from an input character string.
RCHECK	checks the range of the variable to verify that the variable value is between the given bounds.
REDCHR	reads user response to queries that require character string answers.
REDINT	reads user response to queries that require integer answers.
REDREL	reads user response to queries that require real variable answers.
SRTMOL	sorts molecular radiators according to AFGL molecule number.
STUFFD	fills dflts array with regional input information.
UPCASE	converts a character string to all upper case characters.
WRTSTR	writes a character string to an internal file.

ambien.f Major subroutines of the AMBIENT Module

AMBDRV	calls the appropriate subroutines to compute the enhanced vibrationally excited state populations.

ARATE	solves the two-state steady-state equation for the atmospheric excitation rate constant.
CGSUMS	increments Curtis-Godson sums.
COLDEN	computes the total column density for each atmospheric layer for the radiating species.
CPF12	calculates the real part of the complex probability function for a Voigt line shape.
DEWV	computes the equivalent width for a single isolated Voigt line.
DWIDTH	calculates the Doppler halfwidth.
E2	computes the second exponential integral as a function of optical depth.
EMISS	locates the Einstein A coefficient for the current transition, and also calculates the sum of all Einstein A coefficients for all transitions from the upper vibrational state.
ERATE	calculates the earthshine excitation rate for each atmospheric layer.
ESCPRB	normalizes escape probabilities calculated by PATH for each layer.
ESHINE	calculates the earthshine flux for the current transition using the specified effective earthshine temperature.
FORMV	calculates the Voigt line shape function.
GVLOAD	transfers number densities, vibrational transitions, and related information from regional arrays into global ones, which are ultimately used by SPCRAD.
GVZERO	initializes all of the global variable arrays.
LWIDTH	calculates the Lorentz halfwidth.
MULSCT	calculates the nth-order multiple scattering enhancement to the excited-state number density using the single-scattering enhancement matrix.
NEMDRV	is the driver routine to compute the escape probabilities and enhanced excited-state number densities for each atmospheric layer using Monte Carlo integration of atmospheric layers, line strengths, and frequencies.
NEMFAC	computes the probability of escaping a specified layer and the excitation of the layer from all other layers. These quantities are used for the subsequent auroral calculation.
NEMRXN	identifies the excitation and relaxation processes in the chemical kinetics mechanism for the current transition being considered by NEMESIS.
PATH	integrates through the atmospheric layers to determine the escape probabilities and single-scattering enhancements.

PICKSJ	determines the line strength selected from the line strength distribution function.
PICKZ	finds the initial location and the corresponding layer for photon emission.
POPLTE	computes the LTE populations for N_2 and O_2 which are subsequently used in the calculation of vibrationally excited states for CO and H_2O.
N2FAC	computes the effective rate constant for the $CO_2(00011)+N_2(0)$ quenching process and the excited state populations for N_2 following Kumer and James.
QUENCH	computes the total quenching rate for the upper state of the transition.
RANF	is a machine-dependent function which generates uniformly distributed random numbers between 0 and 1.
RVLOAD	transfers the number densities, vibrational transitions, and related information from the local environment arrays into regional arrays.
RVZERO	initializes all regional variable arrays.
SINTRP	performs a linear interpolation to obtain the line strength distribution function for the appropriate layer temperature.
SOLAR	calculates solar flux at a transition frequency assuming a 5500 K blackbody.
SRATE	calculates the solar excitation rate for each atmospheric layer.
STEADY	sets up the steady state rate equations and then uses LUDCMP and LUBKSB to solve the set of linear algebraic equations for the number densities c_k. The major limitation to the steady-state procedure used here is the assumption that the rate equations are linear in the unknown vibrational population, that is, there is no energy exchange among the emitting species. This restriction can be easily relaxed by using an algorithm which solves nonlinear equations (as opposed to LUDCMP/LUBKSB).
VOIGT	determines the emission frequency using a Voigt line shape function. The absorption cross section at this frequency is also computed.

aurora.f — Major subroutines of the AURORAL Module

ALAM	computes Grun's universal energy-dissipation function using a linear interpolation of tabulated values.
AURDRV	is the driver routine for the time-dependent auroral calculation. The auroral species number densities are returned to SHARC main at the observation time specified by the user.

CKLOAD	loads the populations computed during the ambient calculation as the initial number densities for the auroral species.
EPFLUX	calculates the primary energy flux assuming either a Gaussian or Maxwellian distribution function for the electron spectra.
IPPRAT	calculates the ion pair production rate as a function of altitude for the specified auroral energy parameters.
RATMOD	modifies the Einstein A-coefficients and loads the layer excitation rates into the appropriate rate constant arrays. These quantities are computed by the ambient calculation.
TIMDEP	controls the time dependent integration of the auroral rate equations.

chmkin.f CHEMKIN routines for AURORAL Module

ARTCON uses the kinetic data from the auroral linking file to compute the rate constants as a function of temperature in exactly the same manner as RATCON (see below). However, ARTCON identifies primary electron processes and uses the input ionization efficiencies and the ion pair production rate to compute rate constants for secondary electron formation.

CFODE is the alphabetically first of a number of CHEMKIN-derived routines which integrate the differential equations expressing the auroral model. See LSODE.

DAXPY	See LSODE.
DDOT	See LSODE.
DGBFA	See LSODE.
DGBSL	See LSODE.
DGEFA	See LSODE.
DGESL	See LSODE.
DSCAL	See LSODE.
D1MACH	See LSODE.
EWSET	See LSODE.
FUN	supplies LSODE with the species production rates obtained from PRAT.
IDAMAX	See LSODE.

INTDY — See LSODE.

JAC — supplies LSODE with the Jacobian of the species production rates obtained from PRATJ.

LSODE — The LSODE package numerically integrates the auroral rate equations. It uses Gear's method for stiff differential equations and is supplied with the Sandia CHEMKIN code. The following routines are used by the LSODE package:
INTDY, STODE, CFODE, PREPJ, SOLSY, EWSET,
VNORM, DGEFA, DGESL, DGBFA, DGBSL, DAXPY,
DSCAL, DDOT, IDAMAX, DIMACH, XERRWV.

LSODED — See LSODE.

LUDCMP
LUBKSB — are the two subroutines that use a LU decomposition procedure to solve a set of simultaneous linearly independent algebraic equations (the steady-state equations).

PRAT — uses the data obtained from the "linking" file to set up the differential equations for the species production rates.

PRATJ — uses the data obtained from the "linking" file to set up the Jacobian of the species production differential equations with respect to the species number densities.

PREPJ — See LSODE.

RATCON — uses the kinetic data from the linking file to compute the rate constants as a function of temperature. The assumed form of the rate constant is

$$k = A\, T^{\beta} \exp(-E/T - C/T^{1/3}) \quad ,$$

where A is the pre-exponential factor, β is the exponent of the temperature term, E is the activation energy (can also be used to write a reverse rate constant in terms of the forward rate constant via detailed balance), and C is the (historic) SSH $T^{1/3}$ coefficient.

SOLSY — See LSODE.

STODE — See LSODE.

VNORM — See LSODE.

XERRWV — See LSODE. Prints LSODE-related error and warning messages.

geolos.f — INTERACTIVE Module LOS geometry subroutines and geometry utilities

ARCCOS — checks argument of arccosine to make sure it is between 1.0 and -1.0, then computes ACOS.

ARCSIN	checks argument of arcsine to make sure it is between 1.0 and -1.0, then computes ASIN.
ARCTAN	returns an angle between 0 and 2π given the end coordinates of a line that begins at the orgin.
AZI	computes the local azimuth given the latitude of two points and the angle between them.
CHECKG	checks the geometry inputs prior to an calculation.
CONABS	converts a LOS specified in latitudes and longitudes to representation in terms of solar zeniths and azimuths.
CONDTR	converts all angles to radians and transforms coordinates to the geographic coordinate system which is centered at the nort pole.
CONGTM	converts coordinates based on the geographic north pole to magnetic north pole coordinates.
CONMTG	is the inverse of CONGTM.
CONREL	converts a LOS specified in terms of solar zeniths and azimuths to latitude and longitude specifications.
CONRTD	converts all angles to degrees and transforms coordinates to magnetic north pole coordinates.
CROSS	takes the cross product between two vectors using the right hand rule.
DAZI	is a double precision version of AZI.
DLATI	is a double precision version of LATI.
DLONGI	is a double precision version of LONGI.
DOT	takes the dot product of two vectors.
GEOMEX	calculates the full, over-specified set of variables which describe the LOS.
GETAZI	handles interactive input of local azimuth angles for a LOS.
GETLOC	interactively determines a LOS in either latitude, longitude representation or solar zenith, azimuth terms.
GETSOL	handles interactive input of the point beneath the sun in latitude and longitude.
INGEOM	reads LOS geometry information from the default file and allows the user to review/change the parameters.

INSIDE	determines whether the local region forms a proper convex spherical pyramid.
LATI	computes the latitude of point "I" in radians given the latitude of another point, "II" and the latitude of point I to II.
LATPHI	calculates the latitude and longitude of vector 2 relative to vector 1, given the latitudes and longitudes of vectors 1 and 2 relative to a common vector.
LONGI	computes the longitude of point "I" in radians given the longitude of another point, "II" and the longitude of point I to II.
LOS	determines the LOS vector.
MAJSEG	determines the major segments of the LOS through a region.
NORM	normalizes a 3 vector.
OPSANG	computes the supplemental angle.
ORDKEY	determines the relative order of the elements of a vector, and returns an integer vector key containing the element indices in order of increasing element magnitude.
ORDRS	determines the order of occurrence of intersections of the LOS with region boundaries.
PLSECT	determines the intersection of a LOS vector with a plane.
PYRINT	computes segment boundaries of a LOS within a spherical pyramid.
RADE	computes the earth radius as a function of latitude.
RANGER	computes the over-complete set of LOS geometry parameters.
REGANG	maps an arbitrary angle to a specified interval of 2π.
REGDTR	converts edge latitudes and longitudes to radians and converts to geographic coordinates if necessary.
REGLOS	determines if observer or source is inside the angular region.
RELABS	performs interconversion of relative and absolute LOS specifications.
SETGEO	initializes geometry parameters.
SHOGEO	writes the current LOS geometry inputs to the screen.
SHOLOS	writes to the screen all LOS information at the end of a LOS menu session.
SHOZEN	writes to the screen all LOS solar zenith information at end of a menu session.

SUBSOL	computes solar latitude and longitude from the date and time of day, during interactive input.
UNIVEC	determines the unit vector from latitude and longitude.
VECPOL	determines a cartesian vector from an altitude, latitude and longitude.
VECVRT	determines polar coordinates from a cartesian vector.

geoseg.f — Major subroutines of the LOS specification module.

SEGGEN	generates minor segments for each major segment along the specified LOS.
SEGMNT	computes major segment properties, including the major segment lengths, the number of major segments, and identifies the lower boundary for each segment.
PROCAL	calculates the LOS properties for a major segment in a single region.
ZNFDGE	determines the appropriate profile column densities for each segment of the LOS.

spctra.f — Major subroutines of the Radiation transport Module

BNDCMP	compares the transition of a line listed on the HITRAN tape to those specified by the user.
BNDTRN	translates the bands selected by the user to HITRAN nomenclature.
EWV	computes the equivalent width for a single isolated Voigt line.
LINRD	reads the binary line parameter file, one line at a time.
PRTROT	calculates the rotational partition function.
ROT	calculates the LOS radiance for a pure rotational line.
ROTVIB	calculates the LOS radiance for a ro-vibrational line.
SPCRAD	is the main spectral radiance routine called by the main SHARC routine. It calls LINRD to read an individual line, calls BNDCMP to determine if this line is for a user-selected transition, and calls ROT/ROTVIB to perform the LOS radiance calculation. The end result from SPCRAD is the spectral radiance for a line which is stored in array RADBIN.
VIBES	converts vibrational assignments in the HITRAN 92 format to the 85 format when ICHOIC=1. When ICHOIC=2 it converts 85 formats to the 92 ones. This routine is from the HITRAN line selection program.

output.f	Output subroutines used by the various modules
AMBOUT	prints number densities for ambient molecules.
ATMOUT	prints the atmospheric profile.
AUROUT	prints the time dependent number densities for an auroral calculation.
BANNER	outputs the SHARC banner identifying the run.
BNDOUT	prints the line strength distribution function parameters.
BRDOUT	summarizes the calculated band radiances for each transition. The number of lines used in the radiance calculation is also printed.
GEMOUT	writes out a brief summary of the LOS information to SHARC.OUT.
GENOUT	writes out a brief general description of each regional calculation.
LOWOUT	writes the Curtis-Godson information to the output file.
NEMOUT	prints out some of the inputs used by NEMESIS.
POPOUT	outputs the number densities as a function of altitude for each vibrational state in the mechanism.
RADOUT	outputs the information contained in the molecular states file.
RETOUT	writes a summary of the population file to SHARC.OUT when an old population file is used in a new calculation.
SAVE	writes the population file.
SPCOUT	writes the spectral radiance as a function of wavenumber to SHARC.SPC.
SUMOUT	prints a calculational summary at the beginning of each SHARC run.
VBTOUT	outputs the vibrational temperatures as a function of altitude for each vibrational state in the mechanism.
VIBTMP	calculates vibrational temperatures of excited- state species.

APPENDIX D

TEST CASES

SHARC-3 is supplied with five test cases to allow the user to check that it has been properly installed, and to demonstrate some of its features. The input files which define these cases are supplied; if the user employs the data files supplied, the resulting calculation outputs should match those shipped for the cases, apart from minor roundoff error. Appendix A lists the files shipped for each case; each has a general output file TESTn.OUT, where n=1-5, a journal file SHARCn.LOG, spectral and transmission files TESTn.SPC and TESTn.TRN, and a defining input file SHARCn.INP. The main points of interest for each case are discussed here.

PREPARATIONS

To prepare for running the test cases, the user should first compile and link the several SHARC-3 FORTRAN source files and, separately, the INTERPRETER source files. Subdirectories "lines", "popdir", "kindir", "outdir", and "atmdir" should be created. The binary.f program must be compiled, linked, and used to generate the binary lines file SHARC.H92 from its ascii equivalent SHARC.ASC. The SHARC.H92 file should be placed in the "lines" subdirectory. All kinetics files should go into the "kindir" directory. The linking files must be created by using the INTERPRETER as explained in Section 7. All atmosphere files should be placed in the "atmdir" subdirectory. The "popdir" and "outdir" subdirectories will initially be empty. If this set of subdirectories is in some way undesirable, the user will need to modify the directory paths in main menu Item 7, as shown in Section 4.2. The INTERPRETER OUTPUT files and the shipped test case files may be placed in any convenient location for comparison with the outputs of the INTERPRETER and SHARC-3 itself. Note that the names of the test case output files will match those of the shipped files, which should therefore be placed where they will not be overwritten.

FIRST TEST CASE

In a departure from the procedures used for the other test cases, the input file of the first test case, SHARC1.INP, should not be copied to SHARC.INP when the first case is run. This input file is contained in the SHARC-3 source code and written when SHARC-3 is run without a SHARC.INP in the same directory as the executable file. This arrangement insures that the user will never lack for an input file upon which to build. Running SHARC-3 and immediately exiting should create this file, which can then be compared with the shipped version. Once the input file is properly generated, the user can run

the test case and, as for all the cases, compare the output files with those shipped. This first case has a nighttime auroral region embedded in an extended ambient region. The selection of radiators, NO and NO^+, permit this case to run in a relatively brief time. The general output file is a relatively modest 175 Kbytes in size. The journal file should be empty, indicating a successful run with no errors or less significant warning or caution messages. Appendix E2 below reproduces the input file and selected parts of the output file.

SECOND TEST CASE

All remaining cases must be run from the supplied SHARCn.INP files, which the user must copy to SHARC.INP, the only input file which SHARC-3 will look for without modification of the code. The second case calculates nighttime emission from all seven supported radiators, although only the major isotopes of CO_2 and H_2O. The journal file notes that a zero population results for one state of CH_4. This case matches Test Case 1 of earlier SHARC releases.

THIRD TEST CASE

The third case is again a nighttime aurora, with CO_2 added as a radiator; NO and NO^+ are calculated as in the first case. This case is used to demonstrate the reuse of population files. The first two cases generate new population files. Being binary, these files cannot be shipped and must be generated on the user's machine. The species population information in them can be reused once generated. The third-case auroral calculation requires both ambient and auroral population files. Instead of being generated anew, however, the ambient file is that created by the second test case. That file, TEST2.POP, must have been previously generated by the second case and left in the popdir subdirectory in order for the third case to run. The third case creates its own auroral population file ATEST3.POP. Except for the reuse of a population file, this case matches Test Case 2 of earlier SHARC releases.

FOURTH TEST CASE

The fourth and fifth test cases demonstrate the use of multiple atmospheric profiles to model the terminator. The atmosphere generator was used to write seven files representing solar zenith angles from 91° to 102°, spaced approximately along a line of sight at high latitudes. The atmosphere names follow the rule "T4Z(integer solar zenith angle).ATM" for ease in organizing the case, but no particular rule is required for multiple-profile calculations. The test case calculates the radiance of O_3, for which concentration is sensitive to solar illumination. The lines of sight for the first three test cases are limb views; the LOS starts and ends at the maximum 300 Km altitude, capturing radiation from the entire

atmosphere above the tangent altitude. In contrast, this test case uses an observer to space LOS; the observer is located at 184 Km and looks downward through the tangent point and back up to 300 Km.

FIFTH TEST CASE

The fifth case also uses seven profiles (presently the maximum for a single region; change NPOPMX in PARMS.H to change this number) to model a terminator LOS. The names follow the rule "TZ5(integer solar zenith angle).ATM". The observer is in about the same location as in the fourth case, slightly higher at 250 Km. The direction of the LOS is in a less northerly direction. The radiator calculated is CO_2. A calculation involving three isotopes and seven regions produces the largest general output file of the five test cases, even though the number of types of information requested to be printed under top menu Item 5 is less than in the first three cases. The 1.3 Mbyte size of this file underscores the fact that turning on many output options can easily result in an output file of unmanageable proportions. Such large files are a consequence of the complexity of atmospheric modeling, not of SHARC-3 in particular. All of the data appearing in this general output file, in particular the state populations and the vibrational temperatures, can be retrieved from the binary population files during the course of a relatively brief LOS calculation after a CHEMKIN/NEMESIS run has generated those files. Requests for more extensive data output can, however, provide information which is calculated during the CHEMKIN/NEMESIS run and not stored in the population file. The initial, pre-NEMESIS CHEMKIN populations, for example, may only be seen by a request for their printout during the initial generation of the population files. Such more extensive data sets can result in much larger output files than those of the test cases.

APPENDIX E

SHARC U.S. STANDARD ATMOSPHERIC PROFILE

SHARC-3 U.S. 1976 STANDARD MODEL ATMOSPHERE, DAY76.ATM

```
ATMOSPHERE NAME MODIFIED ON 6-16-89 -- (MODIFIED MAY 90)
DAY76.ATM
END
NUMBER OF LAYERS
 66
END
DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE
  DAY  1000.
END
SPECIES
N2 O2 O CO2 CO H2O NO O3 H OH CH4
END
ALTITUDES
50  52  54  56  58
60  62  64  66  68
70  72  74  76  78
80  82  84  86  88
90  92  94  96  98
100  102  104  106  108
110  112  114  116  118
120  122  124  126  128
130  132  134  136  138
140  142  144  146  148
150  160  170  180  190
200  210  220  230  240
250  260  270  280  290
300
END
```

TEMPERATURES

270.65	269.0	263.5	258.0	252.5
2.4706E+02	2.4157E+02	2.3607E+02	2.3058E+02	2.2509E+02
2.1959E+02	2.1426E+02	2.1035E+02	2.0643E+02	2.0252E+02
1.9861E+02	1.9470E+02	1.9078E+02	1.8687E+02	1.8687E+02
1.8687E+02	1.8698E+02	1.8774E+02	1.8931E+02	1.9172E+02
1.9508E+02	1.9953E+02	2.0531E+02	2.1289E+02	2.2329E+02
2.4000E+02	2.6400E+02	2.8800E+02	3.1200E+02	3.3600E+02
3.6000E+02	3.8355E+02	4.0622E+02	4.2804E+02	4.4904E+02
4.6927E+02	4.8838E+02	5.0748E+02	5.2519E+02	5.4290E+02
5.5932E+02	5.7573E+02	5.9095E+02	6.0617E+02	6.2028E+02
6.3439E+02	6.9629E+02	7.4757E+02	7.9007E+02	8.2531E+02
8.5456E+02	8.7679E+02	8.9901E+02	9.0739E+02	9.1578E+02
9.3338E+02	9.5099E+02	9.5724E+02	9.6350E+02	9.6976E+02
9.7601E+02				

END

N2 DENSITIES

1.67E+16	1.32E+16	1.04E+16	8.17E+15	6.40E+15
5.0401E+15	3.9179E+15	3.0285E+15	2.3272E+15	1.7774E+15
1.3487E+15	1.0158E+15	7.5547E+14	5.5885E+14	4.1110E+14
3.0067E+14	2.1859E+14	1.5792E+14	1.1335E+14	7.915E+13
5.547E+13	3.8860E+13	2.7150E+13	1.8940E+13	1.3200E+13
9.2100E+12	6.5080E+12	4.6090E+12	3.2730E+12	2.3270E+12
1.6410E+12	1.1580E+12	8.4220E+11	6.2850E+11	4.7940E+11
3.7260E+11	2.9470E+11	2.3680E+11	1.9300E+11	1.5920E+11
1.3260E+11	1.1160E+11	9.4600E+10	8.0800E+10	6.9470E+10
6.0090E+10	5.2250E+10	4.5650E+10	4.0070E+10	3.5310E+10
3.1240E+10	1.7740E+10	1.0700E+10	6.7400E+09	4.3850E+09
2.9250E+09	1.9890E+09	1.3730E+09	9.6000E+08	6.7780E+08
4.8260E+08	3.4590E+08	2.4940E+08	1.8060E+08	1.3140E+08
9.5930E+07				

END

O2 DENSITIES

4.46E+15	3.52E+15	2.78E+15	2.19E+15	1.71E+15
1.3521E+15	1.0510E+15	8.1245E+14	6.2433E+14	4.7682E+14
3.6181E+14	2.7251E+14	2.0267E+14	1.4992E+14	1.1029E+14
8.0661E+13	5.8641E+13	4.2366E+13	3.0310E+13	2.1200E+13
1.4790E+13	1.0270E+13	7.0600E+12	4.8010E+12	3.2300E+12
2.1510E+12	1.4300E+12	9.4340E+11	6.1890E+11	4.0450E+11
2.6210E+11	1.7060E+11	1.1560E+11	8.1200E+10	5.8920E+10
4.3950E+10	3.3600E+10	2.6250E+10	2.0870E+10	1.6830E+10
1.3750E+10	1.1340E+10	9.4440E+09	7.9270E+09	6.7020E+09
5.7020E+09	4.8810E+09	4.1990E+09	3.6310E+09	3.1530E+09
2.7500E+09	1.4600E+09	8.2770E+08	4.9210E+08	3.0310E+08
1.9180E+08	1.2390E+08	8.1450E+07	5.4250E+07	3.6530E+07
2.4820E+07	1.7000E+07	1.1710E+07	8.1100E+06	5.6430E+06
3.9420E+06				

END

O DENSITIES

8.00E+09	8.66E+09	9.41E+09	1.02E+10	1.11E+10
1.2000E+10	1.3291E+10	1.4720E+10	1.6304E+10	1.8058E+10
2.0000E+10	2.4915E+10	3.1037E+10	3.8664E+10	4.8164E+10
6.0000E+10	6.7650E+10	7.6275E+10	8.6000E+10	1.5100E+11
2.4430E+11	3.4340E+11	4.1590E+11	4.4710E+11	4.4760E+11
4.2980E+11	4.0070E+11	3.6190E+11	3.1880E+11	2.7480E+11
2.3030E+11	1.8890E+11	1.5650E+11	1.3050E+11	1.0960E+11
9.2750E+10	7.9250E+10	6.8400E+10	5.9560E+10	5.2290E+10
4.6250E+10	4.1180E+10	3.6880E+10	3.3200E+10	3.0040E+10
2.7290E+10	2.4890E+10	2.2780E+10	2.0920E+10	1.9270E+10
1.7800E+10	1.2380E+10	8.9960E+09	6.7470E+09	5.1810E+09
4.0500E+09	3.2110E+09	2.5730E+09	2.0810E+09	1.6950E+09
1.3880E+09	1.1430E+09	9.4470E+08	7.8340E+08	6.5160E+08
5.4330E+08				

END

CO2 DENSITIES

7.05E+12	5.56E+12	4.39E+12	3.45E+12	2.71E+12
2.0268E+12	1.5755E+12	1.2178E+12	9.3586E+11	7.1474E+11
5.4235E+11	4.0849E+11	3.0380E+11	2.2473E+11	1.6532E+11
1.2091E+11	8.7901E+10	6.3505E+10	4.5582E+10	3.1936E+10
2.2380E+10	1.5679E+10	1.0958E+10	7.6444E+09	5.3303E+09
3.7193E+09	2.5999E+09	1.8222E+09	1.2809E+09	9.0199E+08
6.3096E+08	3.8519E+08	2.4553E+08	1.6228E+08	1.1063E+08
7.7452E+07	5.5552E+07	4.0724E+07	3.0420E+07	2.3095E+07
1.7785E+07	1.3878E+07	1.0934E+07	8.7128E+06	6.9961E+06
5.6699E+06	4.6236E+06	3.7995E+06	3.1382E+06	2.6089E+06
2.1781E+06	9.4394E+05	4.4431E+05	2.2195E+05	1.1589E+05
6.2601E+04	3.4781E+04	1.9643E+04	1.1394E+04	6.6526E+03
3.8811E+03	2.2906E+03	1.3793E+03	8.3449E+02	5.0729E+02
3.0983E+02				

END

H2O DENSITIES

1.12E+11	8.73E+10	6.82E+10	5.26E+10	4.10E+10
3.35E+10	2.60E+10	2.04E+10	1.51E+10	1.09E+10
7.92E+09	5.75E+09	3.87E+09	2.61E+09	1.68E+09
1.06E+09	6.58E+08	3.59E+08	2.03E+08	1.14E+08
6.14E+07	3.44E+07	1.84E+07	1.05E+07	6.34E+06
3.77E+06	2.34E+06	1.42E+06	8.42E+05	4.81E+05
256000.	137000.	66900.	33600.	26000.
20400.	16300.	13300.	10900.	9130.
7710.	6570.	5630.	4880.	4250.
3720.	3280.	2900.	2580.	2310.
2070.	1260.	822.	560.	395.
287.	213.	161.	124.	96.
76.	60.	48.	39.	32.
26.				

END

NO DENSITIES

2.20E+08	1.72E+08	1.34E+08	1.06E+08	8.28E+07
6.4902E+07	5.0625E+07	3.9488E+07	3.1146E+07	2.4842E+07
1.9814E+07	1.6964E+07	1.4523E+07	1.2734E+07	1.1436E+07
1.0269E+07	1.0927E+07	1.1627E+07	1.5138E+07	1.9711E+07
2.5663E+07	3.2704E+07	4.1846E+07	5.2882E+07	6.1872E+07
7.2242E+07	7.5363E+07	7.7797E+07	7.7797E+07	7.8731E+07
7.8731E+07	7.5313E+07	7.3370E+07	7.0153E+07	6.60E+07
6.15E+07	5.60E+07	4.9804E+07	4.3494E+07	3.7780E+07
3.2572E+07	2.7847E+07	2.4532E+07	2.1422E+07	1.8715E+07
1.6325E+07	1.4088E+07	1.2350E+07	1.0999E+07	9.5536E+06
8.1918E+06	4.1238E+06	2.1095E+06	1.2207E+06	804494.187
530173.87	349392.59	230255.04	151741.56	100000.0
65641.976	43088.691	28284.269	18566.353	12187.323
8000.0				

END

CO DENSITIES

9.83E+08	9.13E+08	8.29E+08	7.79E+08	7.44E+08
9.000E+08	1.050E+09	1.250E+09	1.430E+09	1.550E+09
1.680E+09	1.840E+09	1.920E+09	1.960E+09	1.930E+09
1.830E+09	1.680E+09	1.510E+09	1.280E+09	1.000E+09
7.810E+08	6.720E+08	5.100E+08	4.000E+08	3.000E+08
2.230E+08	1.630E+08	1.200E+08	8.760E+07	6.440E+07
4.700E+07	3.590E+07	2.800E+07	2.250E+07	1.840E+07
1.530E+07	1.260E+07	1.060E+07	9.040E+06	7.750E+06
6.830E+06	5.810E+06	5.000E+06	4.320E+06	3.760E+06
3.300E+06	2.910E+06	2.570E+06	2.290E+06	2.050E+06
1.850E+06	1.090E+06	7.000E+05	4.700E+05	2.980E+05
1.950E+05	1.300E+05	9.070E+04	6.570E+04	4.890E+04
3.800E+04	3.020E+04	2.420E+04	1.940E+04	1.580E+04
1.290E+04				

END

O3 DENSITIES

6.64E+10	3.84E+10	2.55E+10	1.61E+10	1.12E+10
7.30E+09	4.80E+09	3.10E+09	1.80E+09	8.70E+08
3.80E+08	1.70E+08	8.20E+07	4.20E+07	3.00E+07
4.00E+07	7.30E+07	9.00E+07	8.60E+07	6.80E+07
4.90E+07	3.40E+07	2.00E+07	1.20E+07	6.10E+06
3.00E+06	1.40E+06	6.60E+05	2.90E+05	1.30E+05
51400.	18900.	7650.	3330.	1560.
767.	442.0	254.0	146.7	84.7
49.0	33.	23.	16.	10.6
7.2	5.4	4.0	3.0	2.2
1.66	.58	.20	7.100E-02	2.500E-02
8.60E-03	4.700E-03	2.600E-03	1.400E-03	7.600E-04
4.80E-04	2.400E-04	1.400E-04	8.100E-05	4.700E-05
2.70E-05				

END

H DENSITIES

3.28E+05	5.28E+05	7.83E+05	1.12E+06	1.72E+06
2.66E+06	4.12E+06	6.24E+06	9.91E+06	1.55E+07
2.30E+07	3.26E+07	4.05E+07	4.37E+07	3.97E+07
3.23E+07	2.31E+07	1.69E+07	1.61E+07	2.98E+07
5.60E+07	6.54E+07	5.95E+07	4.84E+07	3.78E+07
2.87E+07	2.18E+07	1.64E+07	1.26E+07	9.73E+06
7.56E+06	6.41E+06	5.44E+06	4.46E+06	3.48E+06
2.51E+06	2.14E+06	1.82E+06	1.51E+06	1.20E+06
9.12E+05	8.08E+05	7.03E+05	5.98E+05	4.93E+05
3.88E+05	3.37E+05	2.92E+05	2.47E+05	2.02E+05
1.60E+05	7.13E+04	3.45E+04	1.71E+04	8.00E+03
4.08E+03	2.02E+03	1.05E+03	6.10E+02	3.15E+02
1.74E+02	1.03E+02	5.81E+01	3.19E+01	1.78E+01
9.73E+00				

END

OH DENSITIES

1.44E+07	1.32E+07	1.19E+07	1.16E+07	1.14E+07
1.131E+07	1.183E+07	1.238E+07	1.261E+07	1.250E+07
1.239E+07	1.107E+07	9.890E+06	8.015E+06	5.891E+06
4.330E+06	2.451E+06	1.387E+06	6.276E+05	2.269E+05
8.206E+04	3.079E+04	1.155E+04	4.216E+03	1.497E+03
5.660E+02	2.620E+02	1.420E+02	8.680E+01	5.750E+01
4.030E+01	3.000E+01	2.250E+01	1.730E+01	1.370E+01
1.030E+01	8.250E+00	6.720E+00	5.590E+00	4.730E+00
3.980E+00	3.400E+00	2.900E+00	2.520E+00	2.180E+00
1.914E+00	1.684E+00	1.490E+00	1.322E+00	1.182E+00
1.058E+00	6.440E-01	4.160E-01	2.820E-01	1.990E-01
1.444E-01	1.078E-01	8.100E-02	6.240E-02	4.860E-02
3.800E-02	3.020E-02	2.420E-02	1.942E-02	1.578E-02
1.282E-02				

END

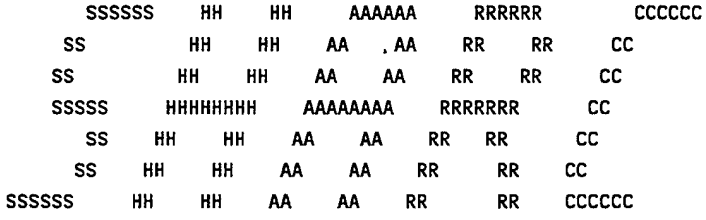
CH4 DENSITIES

4.445E+09	3.189E+09	2.283E+09	1.678E+09	1.264E+09
9.591E+08	7.456E+08	5.763E+08	4.429E+08	3.382E+08
2.567E+08	1.933E+08	1.438E+08	1.064E+08	7.824E+07
5.723E+07	4.161E+07	3.006E+07	2.127E+07	1.447E+07
9.874E+06	6.726E+06	4.570E+06	3.096E+06	2.092E+06
1.415E+06	9.667E+05	6.622E+05	4.499E+05	3.030E+05
2.027E+05	1.200E+05	7.332E+04	4.390E+04	2.566E+04
1.528E+04	8.202E+03	4.473E+03	2.475E+03	1.386E+03
7.840E+02	4.480E+02	2.580E+02	1.497E+02	8.744E+01
5.139E+01	3.037E+01	1.803E+01	1.076E+01	6.447E+00
3.878E+00	3.208E-01	2.828E-02	2.612E-03	2.502E-04
2.464E-05	2.483E-06	2.548E-07	2.656E-08	2.804E-09
2.992E-10	3.224E-11	3.502E-12	3.830E-13	4.214E-14
4.662E-15				

END

APPENDIX F

SHARC OUTPUT FILE
(EXCERPTS FROM TEST CASE 1)



STRATEGIC HIGH-ALTITUDE RADIANCE CODE

VERSION 3.0

********** TEST CASE 1 - NO AND NO+ - TWO REGIONS(AURORAL) **********

1

CALCULATION SUMMARY

NUMBER OF REGIONS: 2

ENVIRONMENT(S) FOR REGION 1:

1 - AMBIENT

USING POPULATION FILE: TEST1.POP

SPECIES-ISOTOPE INPUT FILES:

NO -1 NO.LNK

NO.STA

NO.BND

ENVIRONMENT(S) FOR REGION 2:

2 - AURORAL

USING POPULATION FILE: ATEST1.POP

SPECIES-ISOTOPE INPUT FILES:

NO -1 ANO.LNK

```
                                ANO.STA

                        NO+  -1 ANOP.LNK
                                ANOP.STA


 RADIANCE CALCULATION
  SPECIES-ISOTOPE INCLUDED:     NO   -1
                                NO+  -1
  MINIMUM FREQUENCY:             1500.0 CM-1
  MAXIMUM FREQUENCY:             4000.0 CM-1
  SPECTRAL RESOLUTION:              2.0 CM-1


 SUN LOCATION
  SOLAR LONGITUDE:               180.0 DEG
  SOLAR LATITUDE:                -23.0 DEG

 LINE-OF-SIGHT GEOMETRY
  LOS TYPE:                     LIMB VIEWING PATH
  GEOGRAPHIC POLE COORDINATE SYSTEM
  SPHERICAL EARTH ASSUMED
  LONG PATH   SOURCE RANGE:      3242.5 KM
  TANGENT POINT LOCATION
   TANGENT POINT LOCAL LOS AZIMUTH:  -90.0 DEG
   TANGENT ALTITUDE:             100.0 KM
   TANGENT LONGITUDE:               .0 DEG
   TANGENT LATITUDE:              65.0 DEG
   TANGENT SOLAR ZENITH:         138.0 DEG
   TANGENT SOLAR AZIMUTH:           .0 DEG
  OBSERVER POINT LOCATION
   OBSERVER LOCAL LOS ZENITH ANGLE:  104.1 DEG
   OBSERVER LOCAL LOS AZIMUTH ANGLE: -62.5 DEG
   OBSERVER-EARTH-SOURCE ANGLE:   28.1 DEG
   OBSERVER ALTITUDE:            300.0 KM
   OBSERVER LONGITUDE:            30.7 DEG
   OBSERVER LATITUDE:             61.5 DEG
   OBSERVER SOLAR ZENITH:        136.1 DEG
   OBSERVER SOLAR AZIMUTH:       -20.5 DEG
  SOURCE POINT LOCATION
   SOURCE ALTITUDE:              300.0 KM
   SOURCE LONGITUDE:             329.3 DEG
   SOURCE LATITUDE:               61.5 DEG
   SOURCE SOLAR ZENITH:          136.1 DEG
   SOURCE SOLAR AZIMUTH:          20.5 DEG


1
 AMBIENT ATMOSPHERIC REGION NUMBER  1. PROFILE  1.

  AMBIENT PARAMETERS
```

ATMOSPHERE FILE:	NIG76.ATM
NUMBER OF LAYERS:	65
LOWER BOUNDARY:	50.0 KM
UPPER BOUNDARY:	300.0 KM
EARTHSHINE EXCITATION:	Y
SOLAR ZENITH ANGLE:	138.0
RADIATING SPECIES-ISOTOPE:	NO -1

1

14N 16O RADIATIVE PROPERTIES FOR REGION 1.

STATE	ENERGY(CM-1)	DEGENERACY
NO(0)	.000	1.
NO(1)	1876.077	1.
NO(2)	3724.067	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO(1)	-NO(0)	1876.077	240.0	Y
NO(2)	-NO(0)	3724.067	230.0	Y
NO(2)	-NO(1)	1847.990	240.0	Y

1

14N 16O EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 1.

ALT(KM)	NO(0)	NO(1)	NO(2)
51.0	.196E+09	.801E+04	.389E+00
53.0	.153E+09	.535E+04	.224E+00
55.0	.120E+09	.332E+04	.110E+00
57.0	.944E+08	.204E+04	.535E-01
59.0	.738E+08	.124E+04	.255E-01
61.0	.578E+08	.758E+03	.122E-01
63.0	.451E+08	.464E+03	.582E-02
65.0	.353E+08	.291E+03	.290E-02
67.0	.280E+08	.192E+03	.157E-02
69.0	.223E+08	.134E+03	.938E-03
71.0	.184E+08	.102E+03	.648E-03
73.0	.157E+08	.851E+02	.524E-03
75.0	.136E+08	.743E+02	.459E-03
77.0	.121E+08	.670E+02	.422E-03
79.0	.109E+08	.609E+02	.392E-03
81.0	.106E+08	.592E+02	.388E-03
83.0	.113E+08	.607E+02	.396E-03
85.0	.134E+08	.654E+02	.411E-03
87.0	.174E+08	.733E+02	.426E-03
89.0	.227E+08	.799E+02	.417E-03
91.0	.292E+08	.864E+02	.402E-03

93.0	.373E+08	.978E+02	.416E-03
95.0	.474E+08	.118E+03	.481E-03
97.0	.574E+08	.144E+03	.587E-03
99.0	.671E+08	.178E+03	.745E-03
101.0	.738E+08	.215E+03	.948E-03
103.0	.766E+08	.254E+03	.122E-02
105.0	.778E+08	.310E+03	.167E-02
107.0	.783E+08	.403E+03	.260E-02
109.0	.787E+08	.608E+03	.539E-02
111.0	.770E+08	.112E+04	.175E-01
113.0	.743E+08	.220E+04	.687E-01
115.0	.704E+08	.388E+04	.229E+00
117.0	.643E+08	.603E+04	.620E+00
119.0	.580E+08	.852E+04	.142E+01
121.0	.516E+08	.110E+05	.280E+01
123.0	.449E+08	.131E+05	.475E+01
125.0	.375E+08	.141E+05	.695E+01
127.0	.302E+08	.141E+05	.900E+01
129.0	.243E+08	.135E+05	.109E+02
131.0	.195E+08	.125E+05	.123E+02
133.0	.159E+08	.115E+05	.135E+02
135.0	.131E+08	.105E+05	.145E+02
137.0	.109E+08	.945E+04	.151E+02
139.0	.909E+07	.848E+04	.155E+02
141.0	.776E+07	.768E+04	.158E+02
143.0	.671E+07	.698E+04	.159E+02
145.0	.583E+07	.631E+04	.159E+02
147.0	.507E+07	.566E+04	.156E+02
149.0	.441E+07	.505E+04	.151E+02
155.0	.308E+07	.374E+04	.138E+02
165.0	.155E+07	.188E+04	.903E+01
175.0	.829E+06	.941E+03	.549E+01
185.0	.505E+06	.521E+03	.351E+01
195.0	.333E+06	.305E+03	.229E+01
205.0	.220E+06	.175E+03	.142E+01
215.0	.145E+06	.100E+03	.869E+00
225.0	.954E+05	.561E+02	.508E+00
235.0	.629E+05	.310E+02	.286E+00
245.0	.414E+05	.174E+02	.166E+00
255.0	.271E+05	.995E+01	.997E-01
265.0	.178E+05	.560E+01	.578E-01
275.0	.117E+05	.312E+01	.325E-01
285.0	.768E+04	.174E+01	.184E-01
295.0	.504E+04	.975E+00	.104E-01

1
AURORAL ATMOSPHERIC REGION NUMBER 2. PROFILE 1.

AMBIENT PARAMETERS
ATMOSPHERE FILE: NIG76.ATM

NUMBER OF LAYERS:	65
LOWER BOUNDARY:	50.0 KM
UPPER BOUNDARY:	300.0 KM
EARTHSHINE EXCITATION:	Y
SOLAR ZENITH ANGLE:	138.0
AURORAL PARAMETERS	
MAXWELLIAN ELECTRON ENERGY SPECTRUM	
CODE-SELECTED IBC CLASS:	III
TOTAL ENERGY FLUX:	100.0 ERGS/CM2/SEC
CHARACTERISTIC ENERGY:	5.0 KEV
DURATION OF AURORA:	100.0 SEC
TIME OF OBSERVATION:	100.0 SEC
RADIATING SPECIES-ISOTOPE:	NO -1
	NO+ -1

1

14N 16O RADIATIVE PROPERTIES FOR REGION 2.

STATE	ENERGY(CM-1)	DEGENERACY
NO(0)	.000	1.
NO(1)	1876.077	1.
NO(2)	3724.067	1.
NO(3)	5544.125	1.
NO(4)	7336.086	1.
NO(5)	9100.091	1.
NO(6)	10836.123	1.
NO(7)	12544.098	1.
NO(8)	14223.999	1.
NO(9)	15875.815	1.
NO(10)	17499.535	1.
NO(11)	19095.146	1.
NO(12)	20662.643	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO(1)	-NO(0)	1876.077	240.0	Y
NO(2)	-NO(0)	3724.067	230.0	Y
NO(2)	-NO(1)	1847.990	240.0	Y
NO(3)	-NO(1)	3667.951	240.0	Y
NO(3)	-NO(2)	1819.955	240.0	Y
NO(4)	-NO(2)	3611.916	240.0	Y
NO(4)	-NO(3)	1791.961	240.0	Y
NO(5)	-NO(3)	3555.966	240.0	Y
NO(5)	-NO(4)	1764.005	240.0	Y
NO(6)	-NO(4)	3500.037	240.0	Y
NO(6)	-NO(5)	1736.032	240.0	Y
NO(7)	-NO(5)	3444.007	240.0	Y
NO(7)	-NO(6)	1707.975	240.0	Y

NO(8)	-NO(6)	3387.876	240.0	Y
NO(8)	-NO(7)	1679.901	240.0	Y
NO(9)	-NO(7)	3331.718	240.0	Y
NO(9)	-NO(8)	1651.816	240.0	Y
NO(10)	-NO(8)	3275.536	240.0	Y
NO(10)	-NO(9)	1623.720	240.0	Y
NO(11)	-NO(9)	3219.331	240.0	Y
NO(11)	-NO(10)	1595.611	240.0	Y
NO(12)	-NO(10)	3163.107	240.0	Y
NO(12)	-NO(11)	1567.496	240.0	Y

1

14N 16O EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 2.

ALT(KM)	NO(0)	NO(1)	NO(2)	NO(3)	NO(4)	NO(5)	NO(6)
	NO(7)	NO(8)	NO(9)	NO(10)	NO(11)	NO(12)	
51.0	.196E+09	.801E+04	.389E+00	.000E+00	.000E+00	.000E+00	.000E+00
	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	
81.0	.106E+08	.594E+02	.864E-01	.496E-01	.294E-01	.172E-01	.109E-01
	.648E-02	.381E-02	.195E-02	.954E-03	.428E-03	.138E-03	
83.0	.113E+08	.634E+02	.128E+01	.747E+00	.453E+00	.273E+00	.174E+00
	.105E+00	.623E-01	.320E-01	.158E-01	.715E-02	.233E-02	
85.0	.134E+08	.920E+02	.142E+02	.854E+01	.534E+01	.333E+01	.214E+01
	.131E+01	.787E+00	.407E+00	.202E+00	.927E-01	.306E-01	
87.0	.176E+08	.195E+03	.734E+02	.458E+02	.296E+02	.191E+02	.124E+02
	.776E+01	.469E+01	.245E+01	.122E+01	.568E+00	.189E+00	
89.0	.230E+08	.454E+03	.259E+03	.168E+03	.113E+03	.750E+02	.491E+02
	.314E+02	.192E+02	.101E+02	.507E+01	.238E+01	.803E+00	
91.0	.308E+08	.966E+03	.683E+03	.462E+03	.319E+03	.218E+03	.145E+03
	.938E+02	.579E+02	.307E+02	.155E+02	.737E+01	.251E+01	
93.0	.452E+08	.189E+04	.150E+04	.105E+04	.738E+03	.515E+03	.344E+03
	.226E+03	.141E+03	.751E+02	.381E+02	.183E+02	.624E+01	
95.0	.633E+08	.339E+04	.285E+04	.201E+04	.144E+04	.101E+04	.682E+03
	.451E+03	.282E+03	.151E+03	.771E+02	.371E+02	.127E+02	
97.0	.843E+08	.556E+04	.478E+04	.339E+04	.243E+04	.173E+04	.117E+04
	.774E+03	.485E+03	.261E+03	.133E+03	.643E+02	.221E+02	
99.0	.106E+09	.834E+04	.717E+04	.507E+04	.364E+04	.259E+04	.175E+04
	.116E+04	.730E+03	.392E+03	.200E+03	.969E+02	.335E+02	
101.0	.125E+09	.114E+05	.964E+04	.679E+04	.486E+04	.346E+04	.233E+04
	.155E+04	.973E+03	.523E+03	.267E+03	.129E+03	.447E+02	
103.0	.137E+09	.143E+05	.118E+05	.826E+04	.589E+04	.418E+04	.281E+04
	.187E+04	.117E+04	.628E+03	.321E+03	.155E+03	.538E+02	
105.0	.142E+09	.168E+05	.134E+05	.927E+04	.656E+04	.464E+04	.311E+04
	.206E+04	.129E+04	.692E+03	.353E+03	.171E+03	.593E+02	
107.0	.143E+09	.186E+05	.141E+05	.966E+04	.679E+04	.477E+04	.318E+04
	.211E+04	.132E+04	.705E+03	.359E+03	.174E+03	.604E+02	

109.0	.138E+09	.195E+05	.139E+05	.936E+04	.652E+04	.456E+04	.303E+04
	.200E+04	.125E+04	.666E+03	.339E+03	.164E+03	.571E+02	
111.0	.128E+09	.197E+05	.128E+05	.847E+04	.584E+04	.406E+04	.268E+04
	.176E+04	.110E+04	.586E+03	.297E+03	.144E+03	.502E+02	
113.0	.116E+09	.199E+05	.112E+05	.732E+04	.500E+04	.346E+04	.227E+04
	.149E+04	.927E+03	.494E+03	.250E+03	.121E+03	.422E+02	
115.0	.104E+09	.206E+05	.964E+04	.620E+04	.420E+04	.289E+04	.190E+04
	.124E+04	.769E+03	.409E+03	.207E+03	.100E+03	.350E+02	
117.0	.918E+08	.217E+05	.817E+04	.520E+04	.350E+04	.240E+04	.157E+04
	.102E+04	.634E+03	.337E+03	.170E+03	.823E+02	.288E+02	
119.0	.804E+08	.233E+05	.690E+04	.434E+04	.290E+04	.198E+04	.129E+04
	.843E+03	.521E+03	.277E+03	.140E+03	.675E+02	.236E+02	
121.0	.700E+08	.250E+05	.581E+04	.362E+04	.241E+04	.164E+04	.107E+04
	.695E+03	.429E+03	.228E+03	.115E+03	.555E+02	.194E+02	
123.0	.601E+08	.262E+05	.489E+04	.303E+04	.201E+04	.136E+04	.885E+03
	.575E+03	.355E+03	.188E+03	.950E+02	.458E+02	.160E+02	
125.0	.502E+08	.264E+05	.413E+04	.254E+04	.168E+04	.114E+04	.737E+03
	.478E+03	.295E+03	.156E+03	.788E+02	.380E+02	.133E+02	
127.0	.409E+08	.255E+05	.350E+04	.214E+04	.141E+04	.952E+03	.617E+03
	.400E+03	.246E+03	.130E+03	.658E+02	.317E+02	.111E+02	
129.0	.334E+08	.241E+05	.298E+04	.181E+04	.119E+04	.801E+03	.518E+03
	.336E+03	.207E+03	.109E+03	.552E+02	.266E+02	.932E+01	
131.0	.272E+08	.222E+05	.254E+04	.153E+04	.100E+04	.677E+03	.438E+03
	.283E+03	.174E+03	.922E+02	.465E+02	.224E+02	.785E+01	
133.0	.224E+08	.203E+05	.218E+04	.130E+04	.853E+03	.574E+03	.371E+03
	.240E+03	.147E+03	.780E+02	.393E+02	.190E+02	.665E+01	
135.0	.187E+08	.185E+05	.187E+04	.111E+04	.727E+03	.489E+03	.316E+03
	.204E+03	.125E+03	.663E+02	.334E+02	.161E+02	.565E+01	
137.0	.156E+08	.167E+05	.161E+04	.954E+03	.622E+03	.418E+03	.270E+03
	.174E+03	.107E+03	.565E+02	.285E+02	.137E+02	.481E+01	
139.0	.131E+08	.150E+05	.139E+04	.819E+03	.534E+03	.358E+03	.231E+03
	.149E+03	.915E+02	.484E+02	.244E+02	.117E+02	.412E+01	
141.0	.112E+08	.135E+05	.120E+04	.706E+03	.459E+03	.308E+03	.199E+03
	.128E+03	.787E+02	.416E+02	.209E+02	.101E+02	.354E+01	
143.0	.966E+07	.121E+05	.105E+04	.610E+03	.397E+03	.266E+03	.171E+03
	.111E+03	.678E+02	.358E+02	.180E+02	.869E+01	.305E+01	
145.0	.836E+07	.108E+05	.911E+03	.529E+03	.343E+03	.230E+03	.148E+03
	.956E+02	.586E+02	.310E+02	.156E+02	.751E+01	.264E+01	
147.0	.723E+07	.966E+04	.795E+03	.460E+03	.298E+03	.200E+03	.129E+03
	.829E+02	.508E+02	.268E+02	.135E+02	.651E+01	.229E+01	
149.0	.627E+07	.856E+04	.696E+03	.400E+03	.260E+03	.174E+03	.112E+03
	.721E+02	.442E+02	.233E+02	.118E+02	.566E+01	.199E+01	
155.0	.435E+07	.627E+04	.501E+03	.285E+03	.185E+03	.123E+03	.794E+02
	.512E+02	.313E+02	.166E+02	.834E+01	.401E+01	.141E+01	
165.0	.155E+07	.188E+04	.903E+01	.000E+00	.000E+00	.000E+00	.000E+00
	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	

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14N 16O + RADIATIVE PROPERTIES FOR REGION 2.

STATE ENERGY(CM-1) DEGENERACY

NO+(0)	.000	1.
NO+(1)	2344.160	1.
NO+(2)	4655.668	1.
NO+(3)	6934.433	1.
NO+(4)	9180.356	1.
NO+(5)	11393.349	1.
NO+(6)	13573.319	1.
NO+(7)	15720.170	1.
NO+(8)	17833.813	1.
NO+(9)	19914.141	1.
NO+(10)	21961.072	1.
NO+(11)	23974.510	1.
NO+(12)	25954.361	1.
NO+(13)	27900.529	1.

	TRANSITION	FREQUENCY(CM-1)	ESHINE T(K)	RADIANCE
NO+(1)	-NO+(0)	2344.160	240.0	Y
NO+(2)	-NO+(1)	2311.508	240.0	Y
NO+(3)	-NO+(2)	2278.765	240.0	Y
NO+(4)	-NO+(3)	2245.924	240.0	Y
NO+(5)	-NO+(4)	2212.992	240.0	Y
NO+(6)	-NO+(5)	2179.971	240.0	Y
NO+(7)	-NO+(6)	2146.851	240.0	Y
NO+(8)	-NO+(7)	2113.643	240.0	Y
NO+(9)	-NO+(8)	2080.328	240.0	Y
NO+(10)	-NO+(9)	2046.932	240.0	Y
NO+(11)	-NO+(10)	2013.438	240.0	Y
NO+(12)	-NO+(11)	1979.852	240.0	Y
NO+(13)	-NO+(12)	1946.168	240.0	Y

1

14N 16O + EXCITED STATE NUMBER DENSITIES(MOLEC/CM3) PROFILE 1. REGION 2.

ALT(KM)	NO+(0)	NO+(1)	NO+(2)	NO+(3)	NO+(4)	NO+(5)	NO+(6)
	NO+(7)	NO+(8)	NO+(9)	NO+(10)	NO+(11)	NO+(12)	NO+(13)
81.0	.186E+01	.198E-03	.187E-03	.174E-03	.158E-03	.138E-03	.114E-03
	.880E-04	.573E-04	.447E-04	.437E-04	.403E-04	.297E-04	.178E-04
83.0	.260E+02	.377E-02	.356E-02	.331E-02	.299E-02	.261E-02	.216E-02
	.166E-02	.108E-02	.843E-03	.825E-03	.760E-03	.561E-03	.336E-03
85.0	.234E+03	.459E-01	.432E-01	.401E-01	.361E-01	.315E-01	.260E-01
	.200E-01	.130E-01	.101E-01	.991E-02	.913E-02	.673E-02	.404E-02
87.0	.143E+04	.375E+00	.353E+00	.326E+00	.293E+00	.254E+00	.210E+00
	.161E+00	.105E+00	.814E-01	.795E-01	.732E-01	.540E-01	.324E-01
89.0	.646E+04	.217E+01	.203E+01	.187E+01	.167E+01	.145E+01	.119E+01

	.913E+00	.592E+00	.460E+00	.449E+00	.413E+00	.304E+00	.183E+00
91.0	.229E+05	.923E+01	.855E+01	.782E+01	.696E+01	.600E+01	.492E+01
	.376E+01	.243E+01	.188E+01	.184E+01	.169E+01	.124E+01	.747E+00
93.0	.659E+05	.305E+02	.279E+02	.253E+02	.224E+02	.192E+02	.156E+02
	.119E+02	.767E+01	.593E+01	.577E+01	.530E+01	.390E+01	.234E+01
95.0	.156E+06	.815E+02	.737E+02	.659E+02	.577E+02	.491E+02	.398E+02
	.301E+02	.194E+02	.149E+02	.145E+02	.133E+02	.978E+01	.587E+01
97.0	.613E+06	.183E+03	.162E+03	.143E+03	.123E+03	.104E+03	.835E+02
	.628E+02	.402E+02	.309E+02	.299E+02	.274E+02	.201E+02	.121E+02
99.0	.103E+07	.351E+03	.303E+03	.262E+03	.223E+03	.186E+03	.148E+03
	.111E+03	.703E+02	.538E+02	.520E+02	.475E+02	.349E+02	.209E+02
101.0	.151E+07	.588E+03	.491E+03	.414E+03	.347E+03	.285E+03	.225E+03
	.167E+03	.106E+03	.804E+02	.774E+02	.706E+02	.518E+02	.311E+02
103.0	.196E+07	.874E+03	.701E+03	.576E+03	.473E+03	.384E+03	.300E+03
	.221E+03	.139E+03	.105E+03	.101E+03	.922E+02	.676E+02	.406E+02
105.0	.231E+07	.118E+04	.902E+03	.720E+03	.580E+03	.465E+03	.360E+03
	.263E+03	.164E+03	.124E+03	.119E+03	.108E+03	.793E+02	.476E+02
107.0	.249E+07	.145E+04	.106E+04	.819E+03	.648E+03	.512E+03	.393E+03
	.285E+03	.178E+03	.134E+03	.128E+03	.116E+03	.849E+02	.510E+02
109.0	.248E+07	.163E+04	.113E+04	.852E+03	.663E+03	.518E+03	.394E+03
	.284E+03	.176E+03	.132E+03	.126E+03	.115E+03	.838E+02	.504E+02
111.0	.231E+07	.170E+04	.112E+04	.820E+03	.627E+03	.486E+03	.367E+03
	.264E+03	.163E+03	.122E+03	.116E+03	.105E+03	.770E+02	.463E+02
113.0	.308E+07	.166E+04	.104E+04	.748E+03	.565E+03	.434E+03	.327E+03
	.234E+03	.144E+03	.108E+03	.102E+03	.927E+02	.678E+02	.407E+02
115.0	.269E+07	.156E+04	.940E+03	.664E+03	.498E+03	.380E+03	.285E+03
	.203E+03	.125E+03	.934E+02	.887E+02	.802E+02	.587E+02	.353E+02
117.0	.155E+07	.142E+04	.833E+03	.581E+03	.432E+03	.329E+03	.246E+03
	.175E+03	.108E+03	.802E+02	.762E+02	.689E+02	.504E+02	.303E+02
119.0	.200E+07	.128E+04	.730E+03	.504E+03	.373E+03	.283E+03	.211E+03
	.150E+03	.921E+02	.687E+02	.652E+02	.589E+02	.431E+02	.259E+02
121.0	.171E+07	.114E+04	.635E+03	.436E+03	.321E+03	.243E+03	.181E+03
	.128E+03	.789E+02	.587E+02	.557E+02	.504E+02	.368E+02	.221E+02
123.0	.147E+07	.100E+04	.552E+03	.377E+03	.277E+03	.209E+03	.155E+03
	.110E+03	.677E+02	.504E+02	.478E+02	.432E+02	.316E+02	.190E+02
125.0	.127E+07	.883E+03	.481E+03	.326E+03	.239E+03	.181E+03	.134E+03
	.951E+02	.583E+02	.434E+02	.412E+02	.372E+02	.272E+02	.163E+02
127.0	.110E+07	.777E+03	.419E+03	.283E+03	.207E+03	.156E+03	.116E+03
	.823E+02	.504E+02	.375E+02	.356E+02	.322E+02	.235E+02	.141E+02
129.0	.128E+07	.684E+03	.366E+03	.247E+03	.181E+03	.136E+03	.101E+03
	.715E+02	.438E+02	.326E+02	.309E+02	.279E+02	.204E+02	.123E+02
131.0	.112E+07	.603E+03	.321E+03	.216E+03	.158E+03	.119E+03	.880E+02
	.624E+02	.382E+02	.284E+02	.270E+02	.243E+02	.178E+02	.107E+02
133.0	.981E+06	.533E+03	.282E+03	.190E+03	.138E+03	.104E+03	.771E+02
	.546E+02	.335E+02	.249E+02	.236E+02	.213E+02	.156E+02	.936E+01
135.0	.863E+06	.472E+03	.249E+03	.167E+03	.122E+03	.915E+02	.678E+02
	.480E+02	.294E+02	.219E+02	.207E+02	.187E+02	.137E+02	.822E+01
137.0	.378E+06	.419E+03	.220E+03	.147E+03	.107E+03	.807E+02	.598E+02
	.423E+02	.259E+02	.193E+02	.183E+02	.165E+02	.121E+02	.725E+01
139.0	.334E+06	.372E+03	.195E+03	.130E+03	.950E+02	.714E+02	.529E+02
	.374E+02	.229E+02	.171E+02	.162E+02	.146E+02	.107E+02	.641E+01
141.0	.296E+06	.332E+03	.173E+03	.116E+03	.844E+02	.634E+02	.469E+02

	.332E+02	.203E+02	.151E+02	.143E+02	.130E+02	.946E+01	.569E+01
143.0	.398E+06	.297E+03	.155E+03	.103E+03	.752E+02	.565E+02	.418E+02
	.296E+02	.181E+02	.135E+02	.128E+02	.115E+02	.843E+01	.507E+01
145.0	.356E+06	.265E+03	.138E+03	.923E+02	.671E+02	.504E+02	.373E+02
	.264E+02	.162E+02	.120E+02	.114E+02	.103E+02	.752E+01	.452E+01
147.0	.318E+06	.238E+03	.124E+03	.826E+02	.601E+02	.451E+02	.334E+02
	.236E+02	.145E+02	.108E+02	.102E+02	.922E+01	.673E+01	.405E+01
149.0	.285E+06	.214E+03	.111E+03	.742E+02	.539E+02	.405E+02	.300E+02
	.212E+02	.130E+02	.966E+01	.916E+01	.827E+01	.604E+01	.363E+01
155.0	.290E+06	.164E+03	.849E+02	.566E+02	.412E+02	.309E+02	.229E+02
	.162E+02	.990E+01	.736E+01	.698E+01	.630E+01	.460E+01	.277E+01

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1
LINE-OF-SIGHT GEOMETRY INFORMATION

MAJOR SEGMENT NUMBER 1 TEST1.POP
INITIAL SMALL SEGMENT NO.: 1
ALTITUDE: 300.0 KM
LONGITUDE: 30.7 DEG
LATITUDE: 61.5 DEG
SOLAR ZENITH: 136.1 DEG
RANGE: .0 KM
FINAL SMALL SEGMENT NO.: 32
ALTITUDE: 117.9 KM
LONGITUDE: 10.0 DEG
LATITUDE: 64.7 DEG
SOLAR ZENITH: 137.8 DEG
RANGE: 1139.0 KM

SEGMENT	LOWER ALT.(KM)	UPPER ALT.(KM)	SEGMENT LENGTH(KM)	COLUMN DENSITIES(MOLEC/CM2) NO -1	NO+ -1
1	290.00	300.00	41.65	.2101E+11	.0000E+00
2	280.00	290.00	42.72	.3283E+11	.0000E+00
3	270.00	280.00	43.87	.5128E+11	.0000E+00
4	260.00	270.00	45.13	.8033E+11	.0000E+00
5	250.00	260.00	46.51	.1263E+12	.0000E+00

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29	122.00	124.00	23.79	.1068E+15	.0000E+00
30	120.00	122.00	24.89	.1284E+15	.0000E+00
31	118.00	120.00	26.17	.1518E+15	.0000E+00
32	116.00	118.00	.78	.4748E+13	.0000E+00

32 LAYERS THIS MAJOR SEGMENT
1

LINE-OF-SIGHT GEOMETRY INFORMATION

MAJOR SEGMENT NUMBER 2 ATEST1.POP
INITIAL SMALL SEGMENT NO.: 33
ALTITUDE: 117.9 KM
LONGITUDE: 10.0 DEG
LATITUDE: 64.7 DEG
SOLAR ZENITH: 137.8 DEG
RANGE: 1139.0 KM
FINAL SMALL SEGMENT NO.: 41
ALTITUDE: 100.0 KM
LONGITUDE: 360.0 DEG
LATITUDE: 65.0 DEG
SOLAR ZENITH: 138.0 DEG
RANGE: 1621.2 KM

SEGMENT	LOWER ALT.(KM)	UPPER ALT.(KM)	SEGMENT LENGTH(KM)	COLUMN DENSITIES(MOLEC/CM2)	
				NO -1	NO+ -1
33	116.00	118.00	26.88	.2475E+15	.4215E+13
34	114.00	116.00	29.44	.3072E+15	.7926E+13
35	112.00	114.00	31.62	.3670E+15	.9751E+13
36	110.00	112.00	34.38	.4392E+15	.7952E+13
37	108.00	110.00	38.02	.5243E+15	.9469E+13
38	106.00	108.00	43.14	.6153E+15	.1077E+14
39	104.00	106.00	51.16	.7293E+15	.1183E+14
40	102.00	104.00	66.66	.9111E+15	.1308E+14
41	100.00	102.00	160.89	.2011E+16	.2429E+14

9 LAYERS THIS MAJOR SEGMENT

1
LINE-OF-SIGHT GEOMETRY INFORMATION

MAJOR SEGMENT NUMBER 3 ATEST1.POP
INITIAL SMALL SEGMENT NO.: 42
ALTITUDE: 100.0 KM
LONGITUDE: .0 DEG
LATITUDE: 65.0 DEG
SOLAR ZENITH: 138.0 DEG
RANGE: 1621.2 KM
FINAL SMALL SEGMENT NO.: 50
ALTITUDE: 117.9 KM
LONGITUDE: 350.0 DEG
LATITUDE: 64.7 DEG
SOLAR ZENITH: 137.8 DEG
RANGE: 2103.4 KM

SEGMENT	LOWER ALT.(KM)	UPPER ALT.(KM)	SEGMENT LENGTH(KM)	COLUMN DENSITIES(MOLEC/CM2)	
				NO -1	NO+ -1
42	100.00	102.00	160.90	.2011E+16	.2429E+14
43	102.00	104.00	66.66	.9111E+15	.1308E+14
44	104.00	106.00	51.16	.7293E+15	.1183E+14
45	106.00	108.00	43.14	.6153E+15	.1077E+14

46	108.00	110.00	38.02	.5243E+15	.9469E+13
47	110.00	112.00	34.38	.4392E+15	.7952E+13
48	112.00	114.00	31.62	.3670E+15	.9751E+13
49	114.00	116.00	29.44	.3072E+15	.7926E+13
50	116.00	118.00	26.88	.2474E+15	.4215E+13

9 LAYERS THIS MAJOR SEGMENT

1

LINE-OF-SIGHT GEOMETRY INFORMATION

MAJOR SEGMENT NUMBER 4 TEST1.POP

INITIAL SMALL SEGMENT NO.: 51

ALTITUDE:	117.9 KM
LONGITUDE:	350.0 DEG
LATITUDE:	64.7 DEG
SOLAR ZENITH:	137.8 DEG
RANGE:	2103.4 KM

FINAL SMALL SEGMENT NO.: 82

ALTITUDE:	300.0 KM
LONGITUDE:	329.3 DEG
LATITUDE:	61.5 DEG
SOLAR ZENITH:	136.1 DEG
RANGE:	3242.5 KM

SEGMENT	LOWER ALT.(KM)	UPPER ALT.(KM)	SEGMENT LENGTH(KM)	COLUMN DENSITIES(MOLEC/CM2) NO -1	NO+ -1
51	116.00	118.00	.78	.4785E+13	.0000E+00
52	118.00	120.00	26.17	.1518E+15	.0000E+00
53	120.00	122.00	24.89	.1284E+15	.0000E+00
54	122.00	124.00	23.79	.1068E+15	.0000E+00
55	124.00	126.00	22.82	.8559E+14	.0000E+00

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78	250.00	260.00	46.51	.1263E+12	.0000E+00
79	260.00	270.00	45.13	.8033E+11	.0000E+00
80	270.00	280.00	43.87	.5128E+11	.0000E+00
81	280.00	290.00	42.72	.3283E+11	.0000E+00
82	290.00	300.00	41.65	.2101E+11	.0000E+00

32 LAYERS THIS MAJOR SEGMENT

1

BAND RADIANCE SUMMARY (1500.00 - 4000.00 1/CM)

ISOTOPE	TRANSITION		FREQUENCY(CM-1)	NUMBER OF EMISSION LINES THICK	THIN	TOTAL	BAND RADIANCE (W/SR/CM2)
1	NO(1)	-NO(0)	1876.077	20	620	640	.87186E-07
	NO(2)	-NO(0)	3724.067	100	111	211	.53840E-08
	NO(2)	-NO(1)	1847.990	17	615	632	.79171E-07
	NO(3)	-NO(1)	3667.951	97	114	211	.54973E-08

	NO(3)	-NO(2)	1819.955	14	608	622	.76368E-07
	NO(4)	-NO(2)	3611.916	105	106	211	.11360E-07
	NO(4)	-NO(3)	1791.961	8	606	614	.66315E-07
	NO(5)	-NO(3)	3555.966	103	108	211	.12442E-07
	NO(5)	-NO(4)	1764.005	0	603	603	.54085E-07
	NO(6)	-NO(4)	3500.037	101	110	211	.12160E-07
	NO(6)	-NO(5)	1736.032	0	581	581	.40213E-07
	NO(7)	-NO(5)	3444.007	96	115	211	.10478E-07
	NO(7)	-NO(6)	1707.975	0	555	555	.28894E-07
	NO(8)	-NO(6)	3387.876	88	123	211	.83606E-08
	NO(8)	-NO(7)	1679.901	0	530	530	.19072E-07
	NO(9)	-NO(7)	3331.718	77	134	211	.55245E-08
	NO(9)	-NO(8)	1651.816	0	501	501	.10580E-07
	NO(10)	-NO(8)	3275.536	65	146	211	.33789E-08
	NO(10)	-NO(9)	1623.720	0	471	471	.54933E-08
	NO(11)	-NO(9)	3219.331	46	165	211	.19257E-08
	NO(11)	-NO(10)	1595.611	0	438	438	.26683E-08
	NO(12)	-NO(10)	3163.107	9	202	211	.77801E-09
	NO(12)	-NO(11)	1567.496	0	400	400	.90635E-09
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BAND PASS RADIANCE				946	7962	8908	.54824E-06

1	NO+(1)	-NO+(0)	2344.160	30	51	81	.42684E-08
	NO+(2)	-NO+(1)	2311.508	31	50	81	.55946E-08
	NO+(3)	-NO+(2)	2278.765	31	50	81	.60255E-08
	NO+(4)	-NO+(3)	2245.924	29	52	81	.59019E-08
	NO+(5)	-NO+(4)	2212.992	25	56	81	.54059E-08
	NO+(6)	-NO+(5)	2179.971	23	58	81	.46056E-08
	NO+(7)	-NO+(6)	2146.851	19	62	81	.36086E-08
	NO+(8)	-NO+(7)	2113.643	3	78	81	.23682E-08
	NO+(9)	-NO+(8)	2080.328	0	81	81	.18466E-08
	NO+(10)	-NO+(9)	2046.932	0	81	81	.17970E-08
	NO+(11)	-NO+(10)	2013.438	0	81	81	.16417E-08
	NO+(12)	-NO+(11)	1979.852	0	81	81	.11943E-08
	NO+(13)	-NO+(12)	1946.168	0	81	81	.70402E-09
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BAND PASS RADIANCE				191	862	1053	.44962E-07

TOTAL OVERLAP CORRECTED BAND PASS RADIANCE(1500.00- 4000.00 1/CM) .59318E-06